

## 90494 Access DB#\_ SEARCH REQUEST FORM Scientific and Technical Information Center

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Art Unit: 10 H	Phone N	Number 305 - 6889	Serial Number:	10/070,36/	TNACAU
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Inventors (please pro	ovide full names):	Andrew t	peaton et al	<u> </u>	
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14 APR 2003 HIGHEST RN 502958-40-9 STRUCTURE FILE UPDATES: 14 APR 2003 HIGHEST RN 502958-40-9 DICTIONARY FILE UPDATES:

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002 -

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Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS L9

139256-07-8 REGISTRY

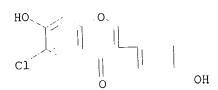
4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) RNCN INDEX NAME)

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C15 H9 C1 O4 MF

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BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER STN Files: LC (\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

5 REFERENCES IN FILE CAPLUS (1962 TO DATE)

1: 137:242178 REFERENCE

137:88466 2: REFERENCE

134:207652 3: REFERENCE

122:187165 4: REFERENCE

5: 116:105915 REFERENCE

Jan Delaval Reference Librarian Biotechnology & Chemical Library CM1 1507 - 703-308-4498 in et aval@uspto.gov

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FILE 'HCAOLD' ENTERED AT 11:22:22 ON 15 APR 2003

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FILE 'USPATFULL, USPAT2' ENTERED AT 11:22:25 ON 15 APR 2003 L11

FILE 'HCAPLUS' ENTERED AT 11:22:31 ON 15 APR 2003

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3 S L12 AND NOVOGEN?/PA,CS L14

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FILE 'REGISTRY' ENTERED AT 11:23:46 ON 15 APR 2003

=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 11:23:56 ON 15 APR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 15 Apr 2003 VOL 138 ISS 16 FILE LAST UPDATED: 14 Apr 2003 (20030414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L15 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2003 ACS
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2002:736111 HCAPLUS AN

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Isoflavone compounds for inhibition of endothelial cell adhesion molecules and treatment of restenosis and other cardiovascular conditions TI

ΤN

Husband, Alan; Kelly, Graham Edmund Novogen Research Pty. Ltd., Australia PΑ

PCT Int. Appl., 100 pp. SO

CODEN: PIXXD2

Patent DT

English LA

ICM A61K031-352 ICS A61P009-10 IC

1-8 (Pharmacology)

Section cross-reference(s): 63

FAN.CNT 1

APPLICATION NO. DATE KIND DATE PATENT NO. \_\_\_\_\_ -----

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20020315
                                           WO 2002-AU288
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
PI WO 2002074307
            W:
            RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                             20010316
PRAI AU 2001-3770
                       A
                            20010626
     AU 2001-5926
     A method is provided for inhibiting expression or activity of an adhesion
     mol. assocd. with an endothelial cell by contacting the adhesion mol. or
     endothelial cell with one or more isoflavone compds. or derivs. thereof.
     Also provided are a method of preventing or reducing the risk of
      restenosis after angioplasty, and a method for the treatment or
      prophylaxis of atherosclerosis, coronary artery diseases, other
      cardiovascular diseases, and inflammatory diseases mediated by adhesion
      mols. The invention further provides pharmaceutical compns. useful in
      these methods, as well as methods for the manuf. of such medicaments.
      isoflavone endothelial cell adhesion mol inhibition; restenosis
      angioplasty cardiovascular disease inflammation isoflavone;
      atherosclerosis coronary artery disease isoflavone
      RL: BSU (Biological study, unclassified); BIOL (Biological study)
 ΙT
         (E-; isoflavone compds. for inhibition of endothelial cell adhesion
         mols. and treatment of restenosis and other cardiovascular conditions)
      RL: BSU (Biological study, unclassified); BIOL (Biological study)
 ΙT
          (LDL; isoflavone compds. for inhibition of endothelial cell adhesion
         mols. and treatment of restenosis and other cardiovascular conditions)
       Cell adhesion molecules
       RL: BSU (Biological study, unclassified); BIOL (Biological study)
  ΙT
          (VCAM-1; isoflavone compds. for inhibition of endothelial cell adhesion
         mols. and treatment of restenosis and other cardiovascular conditions)
          (angina pectoris; isoflavone compds. for inhibition of endothelial cell
       Heart, disease
  ΙT
          adhesion mols. and treatment of restenosis and other cardiovascular
          conditions)
          (angioplasty, restenosis after; isoflavone compds. for inhibition of
  IT
          endothelial cell adhesion mols. and treatment of restenosis and other
          cardiovascular conditions)
           (antiatherosclerotics; isoflavone compds. for inhibition of endothelial
       Antiarteriosclerotics
  IT
          cell adhesion mols. and treatment of restenosis and other
           cardiovascular conditions)
           (atherectomy, direction coronary atherectomy; isoflavone compds. for
       Artery
   TT
           inhibition of endothelial cell adhesion mols. and treatment of
           restenosis and other cardiovascular conditions)
           (coronary; isoflavone compds. for inhibition of endothelial cell
        Artery, disease
   ΙT
           adhesion mols. and treatment of restenosis and other cardiovascular
           conditions)
           (endothelium; isoflavone compds. for inhibition of endothelial cell
        Blood vessel
  IT
           adhesion mols. and treatment of restenosis and other cardiovascular
           conditions)
        Lipoproteins
   IT
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conditions)

Surgery

RL: BSU (Biological study, unclassified); BIOL (Biological study) (high-d.; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Anti-inflammatory agents Antihypertensives Antioxidants Atherosclerosis Blood vessel, disease Cardiovascular agents Cell migration Cytotoxic agents Drug delivery systems Human Hypertension Inflammation Transplant and Transplantation Vasodilators (isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Cell adhesion molecules RL: BSU (Biological study, unclassified); BIOL (Biological study) (isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Flavones RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (isoflavones; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Lipoproteins RL: BSU (Biological study, unclassified); BIOL (Biological study) (low-d., oxidized; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Lipoproteins RL: BSU (Biological study, unclassified); BIOL (Biological study) (low-d.; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Blood vessel (procedural vascular trauma; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Artery, disease (restenosis; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Blood vessel, disease (small vessel disease; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Blood vessel (smooth muscle; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Medical goods (stents; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) (surgery; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular

(vascular; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

23531-69-3, .alpha.-Tocopheroxyl radical 1406-18-4, Vitamin E RL: BSU (Biological study, unclassified); BIOL (Biological study) IT (isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) 21255-69-6

17238-05-0 486-66-8 491-80-5 485-72-3 446-72-0 81267-65-4 81267-63-2 IT 62845-21-0 40957-83-3, Glycitein 21554-71-2 153409-51-9 145917-93-7 94105-90-5 139256-07-8 88040-00-0 288267-04-9 288267-03-8 288267-00-5 168207-16-7 168207-15-6 351216-89-2, 328406-49-1 328406-47-9 328406-44-6 288267-05-0 442150-46-1 Promensil 442150-42-7 442150-43-8 442150-44-9 442150-61-0 442150-54-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT

(1) G J Consultants Pty Ltd; WO 0066576 A 2000 HCAPLUS

(2) Johnson & Johnson Consumer Companies Inc; WO 0054753 A 2000 HCAPLUS

(3) Kelly, S; American Journal of Physiology 1998, V274(2 Pt 2), PH513 MEDLINE

(4) May, M; Journal of Pharmacology 1996, V118(7), P1761 HCAPLUS

(5) Novogen Research Pty Ltd; WO 0064438 A 2000 HCAPLUS

(6) Palmetshofer, A; Transplantation 1998, V65(7), P971 HCAPLUS

(7) Protein Technologies InternationalInc; AU 2771400 A1 2000

(8) Schnyder; WO 0016759 A 2000 HCAPLUS

(9) Weber, C; Immunologic research 1996, V15(1), P30 HCAPLUS

139256-07-8 ΙT

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) 139256-07-8 HCAPLUS RN CN INDEX NAME)

L15 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS

2002:539523 HCAPLUS ΑN

DN

Isoflavones in combination with lipid-regulating agents for regulation of lipids and/or bone density, and compositions therefor TΙ

Husband, Alan James

INNovogen Research Pty Ltd., Australia

PΑ PCT Int. Appl., 45 pp. SO

CODEN: PIXXD2

Patent DT

English LA IC

ICS A61K031-352; A61K035-78; A61K031-465; A61P009-10; A61P019-10

1-10 (Pharmacology) CC Section cross-reference(s): 63

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                                          APPLICATION NO. DATE
                     KIND DATE
    PATENT NO.
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                                          WO 2002-AU42
                            20020718
    WO 2002055072
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                            20010116
PRAI AU 2001-2554
     MARPAT 137:88466
     A method and compns. are provided for regulating bone d. and/or
     circulating lipid levels in a subject which are based on the combined
     administration of at least one isoflavone, or functional deriv., equiv.,
     or analog thereof, and at least one lipid-regulating drug. The method and
     compns. are applicable to the beneficial alteration of blood lipoprotein
     levels, the improvement of vascular compliance, the decrease in the
     propensity of thrombogenic events, the redn. in the risk of vascular
     disease, coronary heart disease, and arteriosclerosis, and to the
     treatment or prevention of osteoporosis.
     cardiovascular drug isoflavone lipid regulating agent combination;
ST
     osteoporosis drug isoflavone lipid regulating agent combination; bone
     density drug isoflavone lipid regulating agent combination; lipid
     regulation agent isoflavone combination
     Sequestering agents
ΙT
        (bile acid-binding; isoflavone combination with lipid-regulating agent
        for regulation of lipids and/or bone d.)
     Artery, disease
IT
        (coronary; isoflavone combination with lipid-regulating agent for
        regulation of lipids and/or bone d.)
ΙT
        (d.; isoflavone combination with lipid-regulating agent for regulation
        of lipids and/or bone d.)
ΙT
     Lipoproteins
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (high-d., cholesterol; isoflavone combination with lipid-regulating
        agent for regulation of lipids and/or bone d.)
     Lipids, biological studies
IT
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (hyperlipidemia; isoflavone combination with lipid-regulating agent for
         regulation of lipids and/or bone d.)
      Heart, disease
IT
         (ischemia; isoflavone combination with lipid-regulating agent for
         regulation of lipids and/or bone d.)
      Anti-ischemic agents
 TΤ
      Antiarteriosclerotics
      Anticholesteremic agents
      Anticoagulants
      Arteriosclerosis
      Blood vessel, disease
      Cardiovascular agents
      Drug delivery systems
      Hypercholesterolemia
      Hypolipemic agents
      Osteoporosis
      Thrombosis
         (isoflavone combination with lipid-regulating agent for regulation of
         lipids and/or bone d.)
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Lipids, biological studies RL: BSU (Biological study, unclassified); BIOL (Biological study) ΙT (isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) Flavones RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL ΙT (Biological study); USES (Uses) (isoflavones; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) Lipoproteins RL: BSU (Biological study, unclassified); BIOL (Biological study) IT (low-d., cholesterol; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) RL: BSU (Biological study, unclassified); BIOL (Biological study) IT (resins binding; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) Drug interactions (synergistic; isoflavone combination with lipid-regulating agent for ΙT regulation of lipids and/or bone d.) (therapeutic agents; isoflavone combination with lipid-regulating agent Osteoporosis IT for regulation of lipids and/or bone d.) Glycerides, biological studies ΙT RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (.omega.-3; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) 9028-35-7, HMG-CoA reductase RL: BSU (Biological study, unclassified); BIOL (Biological study) ΙT (inhibitors; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) 57-88-5, Cholesterol, biological studies RL: BSU (Biological study, unclassified); BIOL (Biological study) ΙT (isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) 59-67-6D, Nicotinic acid, 59-67-6, Nicotinic acid, biological studies ΙT 485-72-3 446-72-0D, analogs and derivs. 446-72-0 486-66-8D, analogs and derivs. 486-66-8 485-72-3D, analogs and derivs. 897-46-1D, analogs 897-46-1 491-80-5D, analogs and derivs. 491-80-5 17238-05-0D, 17238-05-0 943-45-3D, Fibric acid, derivs. and derivs. 17817-31-1D, analogs and derivs. 17817-31-1 analogs and derivs. 21554-71-2D, 21554-71-2 21255-69-6D, analogs and derivs. 21255-69-6 62845-21-0D, analogs and derivs. 62845-21-0 analogs and derivs. 76397-85-8D, analogs and derivs. 76397-85-8 75330-75-5, Lovastatin 79902-63-9, Simvastatin 76397-87-0D, analogs and derivs. 76397-87-0 81267-63-2D, analogs and derivs. 81267-63-2 81093-37-0, Pravastatin 88040-00-0D, 81267-65-4D, analogs and derivs. 88040-00-0 81267-65-4 94105-87-0D, 94105-87-0 93957-54-1, Fluvastatin analogs and derivs. 94105-89-2D, analogs and derivs. 94105-89-2 analogs and derivs. 134523-00-5, Atorvastatin 94105-90-5D, analogs and derivs. 94105-90-5 139256-07-8 139256-07-8D, analogs and derivs. 145917-92-6D, analogs and 145917-92-6 145599-86-6, ·Cerivastatin 145917-93-7D, analogs and derivs.  $1\overline{5}3409-51-9$ 145917-93-7 derivs. 168207-15-6D, analogs 168207-15-6 153409-51-9D, analogs and derivs. 168207-16-7D, analogs and derivs. 168207-16-7 and derivs. 288267-03-8 288267-00-5D, analogs and derivs. 288267-00-5 288267-04-9D, analogs 288267-04-9 288267-03-8D, analogs and derivs. 288267-05-0D, analogs and derivs. 288267-05-0 and derivs. 328406-44-6D, analogs and derivs. 328406-47-9 328406-44-6 328406-49-1D, analogs 328406-49-1 328406-47-9D, analogs and derivs. 442150-42-7D, analogs 442150-42-7 351217-32-8, Trinovin and derivs. 442150-43-8D, analogs and derivs. 442150-43-8

and derivs.

442150-44-9D, analogs and derivs. 442150-46-1 442150-44-9 442150-46-1D, analogs and derivs. 442150-54-1 442150-54-1D, analogs 442150-61-0D, analogs and derivs. 442150-61-0 and derivs. 442150-68-7D, analogs and derivs. 442150-70-1 442150-68-7 442150-70-1D, analogs and derivs. RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT RE (1) Bristol-Myers Squibb Company; AU 1022795 A 1995 (2) Bristol-Myers Squibb Company; EP 671170 A 1995 HCAPLUS (3) Kelly, G; WO 9323069 A 1993 HCAPLUS (4) Novogen Research Pty Ltd; WO 0064438 A 2000 HCAPLUS (5) Pfizer Inc; WO 9911260 A 1999 HCAPLUS (6) Pfizer Products Inc; WO 9911263 A 1999 HCAPLUS (7) Potter, S; US 5855892 A 1999 HCAPLUS 139256-07-8 139256-07-8D, analogs and derivs. ΤТ RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (isoflavone combination with lipid-regulating agent for regulation of

139256-07-8 HCAPLUS RN

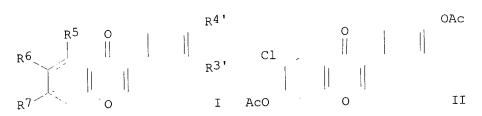
lipids and/or bone d.)

4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) CN INDEX NAME)

139256-07-8 HCAPLUS RN 4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA CN INDEX NAME)

- ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS L15
- 2001:185742 HCAPLUS ΑN
- DN 134:207652
- Preparation of isoflavones as therapeutic agents with estrogen receptor TIbinding activity
- Heaton, Andrew; Kumar, Naresh; Kelly, Graham ΙN Edmund; Husband, Alan
- Novogen Research Pty. Ltd., Australia PA
- PCT Int. Appl., 44 pp. SO CODEN: PIXXD2
- DTPatent
- English LA
- ICM C07D311-36 IC

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C07D311-38; C07D471-06; C07C049-215; C07C049-213; A61K031-12;
         A61K031-437; A61P005-00; A61P025-22; A61P025-24; A61P009-10;
          A61P019-10; A61P019-02; A61P017-06; A61P007-00; A61P035-00;
          A61P025-28; A61P017-04; A61P001-00
     26-4 (Biomolecules and Their Synthetic Analogs)
     Section cross-reference(s): 1, 2, 63
FAN.CNT 1
                                                            DATE
                                           APPLICATION NO.
                      KIND DATE
     PATENT NO.
                                           _____
                      ____
                                           WO 2000-AU1056
                                                            20000906
                            20010315
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PΙ
     WO 2001017986
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             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,
                                                         TM
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     EP 1210341
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             IE, SI, LT, LV, FI, RO, MK, CY, AL
                                           JP 2001-522209
                                                             20000906
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                            20030304
     JP 2003508526
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                                                             20020306
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PRAI AU 1999-2661
                       Α
                            20000906
     WO 2000-AU1056
                       W
OS
     MARPAT 134:207652
GT
```



AB Isoflavanoids, such as I [R3', R4', R7 = H, OH, OAc, etc.; R5 = H, OH, OAc, Me, etc.; R6 = H, Cl, etc.], were prepd. for pharmaceutical use in the treatment of diseases assocd. with estrogenic or androgenic effects. Thus, isoflavone II was prepd. in 75% yield by acetylation of 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one with acetic anhydride in pyridine. The prepd. isoflavanoids were tested for binding affinity for both subtypes of the estrogen receptor.

ST isoflavanoid prepn estrogen receptor binding

IT Isoflavonoids

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(prepn. of isoflavones with estrogen receptor binding activity for pharmaceutical use)

IT Estrogen receptors

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(prepn. of isoflavones with estrogen receptor binding activity for pharmaceutical use)

TT 328406-42-4P 328406-43-5P 328406-45-7P 328406-47-9P 328406-50-4P 328406-51-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of isoflavones with estrogen receptor binding activity for pharmaceutical use) 81267-53-0 **139256-07-8** RL: BAC (Biological activity or effector, except adverse); BSU (Biological IT study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses) (prepn. of isoflavones with estrogen receptor binding activity for 328406-44-6P pharmaceutical use) 81267-67-6P 81267-61-0P 65998-44**-**9P 65998-43-8P 328406-48-0P 328406-49-1P IT RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of isoflavones with estrogen receptor binding activity for pharmaceutical use) 328406-52-6 108-73-6, 1,3,5-Benzenetriol RL: RCT (Reactant); RACT (Reactant or reagent) ΙT (prepn. of isoflavones with estrogen receptor binding activity for THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD pharmaceutical use) 14 RE.CNT (1) Anticancer Inc; WO 9848790 Al 1998 HCAPLUS (2) Bannerjee; J Electrochem Soc India 1998, V47(4), P237 HCAPLUS (3) Children'S Hospital Oakland Research Institute; WO 9918953 Al 1999 HCAPLUS (4) Laboratoire L Lafon; WO 0003707 A1 2000 HCAPLUS (5) Lamberton; Aust J Chem 1978, V31(2), P455 HCAPLUS (6) Liepa; Aust J Chem 1981, V34(12), P2647 HCAPLUS (7) Lyonnaise Industrielle Pharmaceutique; FR 2693724 A1 1994 HCAPLUS (8) New Standard Gmbh; DE 4432947 A1 1996 HCAPLUS (9) Novogen Research Pty Ltd; WO 9808503 Al 1998 HCAPLUS (10) Novogen Research Pty Ltd; WO 9936050 Al 1999 HCAPLUS (11) Ota Isan Kk; JP 01226824 A 1989 HCAPLUS (12) Wahala; Heterocycles 1989, V28(1), P183 HCAPLUS (13) Weidenborner; Phytochemistry 1990, V29(3), P801 (14) Zilliken; US 4157984 1979 HCAPLUS RL: BAC (Biological activity or effector, except adverse); BSU (Biological ΤT study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses) (prepn. of isoflavones with estrogen receptor binding activity for pharmaceutical use) 4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA 139256-07-8 HCAPLUS RN CNINDEX NAME)

- L15 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2003 ACS
- 1995:293255 HCAPLUS AN
- Synthesis and labeling of isoflavone phytoestrogens, including daidzein 122:187165 DN TΙ and genistein

```
Waehaelae, Kristina; Hase, Tapio; Adlercreutz, Herman
    Dep. Chemistry, Univ. Helsinki, Helsinki, FIN-00014, Finland
ΑU
    Proceedings of the Society for Experimental Biology and Medicine (1995),
CS
SO
     208(1), 27-32
     CODEN: PSEBAA; ISSN: 0037-9727
PΒ
     Blackwell
     Journal
DT
     English
LΑ
     26-4 (Biomolecules and Their Synthetic Analogs)
     The synthesis of the important diphenolic isoflavone type of
CC
     phytoestrogens starting from the corresponding unprotected phenols and
AΒ
     arylacetic acids is discussed. The aryl rings may carry addnl. alkyl,
     methoxy, and/or halogeno groups. Intermediate polyhydroxydeoxybenzoins
     can also be isolated in good yield. Isotopically labeled isoflavone
     phytoestrogens were prepd. by H/D exchange in the complete mol. By this
     method the deuterated products are available in an isotopic purity of
     isoflavone; arylacetate phenol acylation; deuteration daidzein genistein
ST
     Flavonoids
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (iso-, oxo, prepn. and labeling of isoflavones from phenols and
        arylacetic acids)
     104-01-8, 4-Methoxyphenylacetic acid
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (prepn. and labeling of isoflavones from phenols and arylacetic acids)
                     136466-47-2P
      104411-13-4P
 IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and labeling of isoflavones from phenols and arylacetic acids)
                                    93-25-4, 2-Methoxyphenylacetic acid
      87-66-1, 1,2,3-Benzenetriol
                                         103-82-2, Phenylacetic acid, reactions
 IT
      95-88-5, 4-Chloro-1,3-benzenediol
                                            108-46-3, 1,3-Benzenediol, reactions
      106-44-5, 4-Methylphenol, reactions
                                                                    120-80-9,
                                     108-95-2, Phenol, reactions
      108-73-6, 1,3,5-Benzenetriol
                                  156-38-7, 4-Hydroxyphenylacetic acid
      1,2-Benzenediol, reactions
      306-08-1, 4-Hydroxy-3-methoxyphenylacetic acid
                                                        504-15-4,
                                 533-73-3, 1,3,4-Benzenetriol 608-25
614-75-5, 2-Hydroxyphenylacetic acid
                                                                 608-25-3,
      5-Methyl-1,3-benzenediol
      2-Methyl-1, 3-benzenediol
                                             1798-09-0, 3-Methoxyphenylacetic
      621-37-4, 3-Hydroxyphenylacetic acid
      acid
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (prepn. of isoflavones from phenols and arylacetic acids)
                                                         15485-65-1P
                               2491-32-9P
                                             3669-41-8P
                 2491-31-8P
      487-49-0P
 TΨ
                                                89019-83-0P
                                                              89019-84-1P
                                   77316-95-1P
                    40456-49-3P
      17720-60-4P
                                                                  150295-88-8P
                                                  139256-04-5P
                                   139256-03-4P
                    139256-02-3P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
       (Reactant or reagent)
          (prepn. of isoflavones from phenols and arylacetic acids)
                             485-72-3P, 7-Hydroxy-4 -methoxyisoflavone
       446-72-0P, Genistein
                             491-80-5P, 5,7-Dihydroxy-4'-methoxyisoflavone
 TΤ
       486-66-8P, Daidzein
                                                                      13057-72-2P,
                               4044-00-2P, 5,7-Dihydroxyisoflavone
       574-12-9P, Isoflavone
                                                        62845-21-0P
                                           21913-98-4P
                             19725-36-1P
       7-Hydroxyisoflavone
       63909-40-0P, 7-Hydroxy-2'-methoxyisoflavone
                                                                   89019-85-2P
                                                     75187-63-2P
                                    139256-06-7P 139256-07-8P
                      139256-05-6P
       118024-87-6P
       139256-08-9P
       RL: SPN (Synthetic preparation); PREP (Preparation)
          (prepn. of isoflavones from phenols and arylacetic acids)
       139256-07-8P
  TΨ
       RL: SPN (Synthetic preparation); PREP (Preparation)
          (prepn. of isoflavones from phenols and arylacetic acids)
       139256-07-8 HCAPLUS
       4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI)
  RN
  CN
       INDEX NAME)
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HO.
          0
                       ОН
    ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS
     1992:105915 HCAPLUS
ΑN
     116:105915
DN
     Expedient synthesis of polyhydroxyisoflavones
ΤI
     Wahala, Kristiina; Hase, Tapio A.
     Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
ΑU
     Journal of the Chemical Society, Perkin Transactions 1: Organic and
CS
SO
     Bio-Organic Chemistry (1972-1999) (1991), (12), 3005-8
     CODEN: JCPRB4; ISSN: 0300-922X
     Journal
DT
     English
LA
      26-4 (Biomolecules and Their Synthetic Analogs)
CC
      CASREACT 116:105915
      Polyhydroxyisoflavones (19 compds.) were prepd. by reaction of unprotected
OS
      phenols with arylacetic acid in the presence of BF3. Et20 followed by
 AΒ
      treatment with MeSO2Cl. In many cases the intermediate deoxybenzoins were
      also isolated.
```

isoflavone polyhydroxy; deoxybenzoin polyhydroxy; phenol arylacetate STcondensation

Flavonoids IT

RL: SPN (Synthetic preparation); PREP (Preparation) (iso-, hydroxy oxo, polyhydroxy-, prepn. of, from unprotected phenols and arylacetic acids)

1835-11-6 ΙT

RL: RCT (Reactant); RACT (Reactant or reagent) (oxidn. of)

15485-65-1P 3669-41-8P 2491-31-8P 2491-32-9P 487-49-0P 77316-95-1P 89019-83-0P ΙT 52122-86-8P 40456-49-3P 17720-60-4P 139256-03-4P 139256-02-3P 139256-01-2P 92549-46-7P 89019-84-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and intramol. cyclocondensation of)

ΙT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, with phenols)

67736-18-9P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

574-12-9P, Isoflavone 491-80-5P 486-66-8P 485-72-3P 446-72-0P TΤ 32684-57-4P 21913-98-4P 19725-36-1P 13057-72-2P 4044-00-2P 118024-87-6P 89019-85-2P 75187-63-2P 63909-40-0P 62845-21-0P 139256-08-9P 139256-06-7P **139256-07-8P** 139256-05-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from phenol and phenylacetic acid)

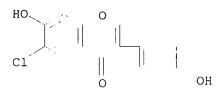
103-82-2, Phenylacetic acid, 93-25-4, 2-Methoxyphenylacetic acid 104-01-8, 4-Methoxyphenylacetic acid 156-38-7, IT 4-Hydroxyphenylacetic acid 614-75-5, 2-Hydroxyphenylacetic acid 621-37-4, 3-Hydroxyphenylacetic acid 1798-09-0, 3-Methoxyphenylacetic 621-37-4, 3-Hydroxyphenylacetic acid acid

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with phenols)

95-88-5, 4-Chloro-1,3-benzenediol 87-66-1, 1,2,3-Benzenetriol IT

106-44-5, p-Cresol, reactions 108-46-3, m-Hydroquinone, reactions 108-73-6, 1,3,5-Benzenetriol 108-95-2, Phenol, reactions 120-80-9, o-Hydroquinone, reactions 123-31-9, p-Hydroquinone, reactions 504-15-4, 5-Methyl-1,3-benzenediol 533-73-3, 1,3,4-Benzenetriol 608-25-3, 2-Methyl-1,3-benzenediol RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with phenylacetic acids) 139256-07-8P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from phenol and phenylacetic acid)

RN 139256-07-8 HCAPLUS CN 4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



ΙT

=> fil reg FILE 'REGISTRY' ENTERED AT 11:47:39 ON 15 APR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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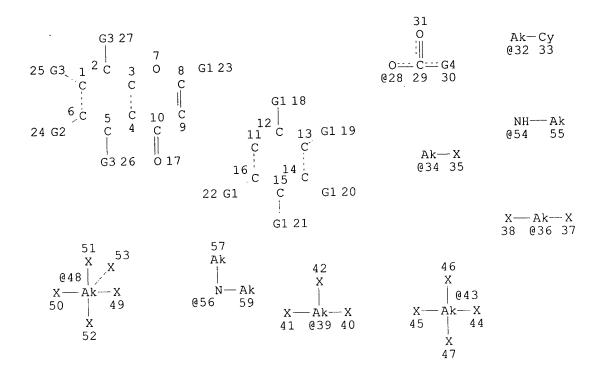
TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting  ${\tt SmartSELECT}$  searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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VAR G1=H/OH VAR G2=H/X VAR G3=H/OH/AK/28 VAR G4=H/AK/34/36/39/43/48/NH2/54/56/32 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 58

STEREO ATTRIBUTES: NONE L18 169 SEA FILE=REGISTRY SUB=L2 CSS FUL L16

100.0% PROCESSED 6958 ITERATIONS 169 ANSWERS SEARCH TIME: 00.00.01

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L2
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L3
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L4
             20 S L3 NOT L4
L5
             16 S L5 NOT 6 CHLORO
L6
              4 S L5 NOT L6
L7
              3 S L7 NOT 7 HYDROXY
\Gamma8
              1 S L7 NOT L8
L9
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L10
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     FILE 'USPATFULL, USPAT2' ENTERED AT 11:22:25 ON 15 APR 2003
L11
     FILE 'HCAPLUS' ENTERED AT 11:22:31 ON 15 APR 2003
L12
              5 S L9
              3 S L12 AND (HEATON ? OR KUMAR ? OR KELLY ? OR HUSBAND ?)/AU
L13
              3 S L12 AND NOVOGEN?/PA,CS
L14
L15
              5 S L12-L14
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     FILE 'HCAPLUS' ENTERED AT 11:23:56 ON 15 APR 2003
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L19
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             11 S L19 AND C15H1006
L20
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L21
L22
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L23
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L24
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L26
           4036 S L24
             21 S L26 AND (HEATON A? OR KUMAR N? OR KELLY G? OR HUSBAND A?)/AU
L27
L28
             12 S L26 AND NOVOGEN?/PA,CS
L29
             21 S L27, L28
           2704 S L26 AND (PD<=19990906 OR PRD<=19990906 OR AD<=19990906)
L30
             14 S L29 AND L30
L31
                E W02000-AU1056/AP, PRN
L32
              1 S E3, E4
L33
              1 S L32 AND L26
                E ESTROGEN RECEPTOR/CT
L34
           8369 S E11-E18
                E E11+ALL
          13813 S E12, E11+NT
L35
L36
             86 S L30 AND L34, L35
             14 S L31, L33
L37
              1 S L37 AND L34, L35
L38
L39
             14 S L37, L38
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L40
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L41
              9 S L40 NOT (GENISTERIN OR DAIDZEOL)/CN
              8 S L41 NOT ISOFLAVONE/CN
L42
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L43
L44
            166 S L43 AND L30
L45
              2 S L44 AND L34, L35
L46
              2 S L44 AND ?ESTROGEN? (L) RECEPTOR
L47
              2 S L45, L46, L33, L38
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45 S L44 AND P/DT
L48
              18 S L48 AND US/PC
L49
              19 S L47, L49
L50
     FILE 'REGISTRY' ENTERED AT 11:47:39 ON 15 APR 2003
=> d ide can 121
L21 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
      480-23-9 REGISTRY
      4H-1-Benzopyran-4-one, 3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-
RN
CN
      (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
      Isoflavone, 3',4',5,7-tetrahydroxy- (7CI, 8CI)
OTHER NAMES:
      3',4',5,7-Tetrahydroxyisoflavone
      5,7,3',4'-Tetrahydroxyisoflavone
CN
      Isoluteolin
 CN
      Orobol
 CN
      3D CONCORD
 FS
        N Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CHEMCATS, DDFU, DRUĞU, EMBASE,
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 MF
      STN Files:
 LC
        MEDLINE, NAPRALERT, RTECS*, TOXCENTER, USPATFULL
           (*File contains numerically searchable property data)
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## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

137:226166

94 REFERENCES IN FILE CA (1962 TO DATE) 94 REFERENCES IN FILE CAPLUS (1962 TO DATE) 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

LZI and LZZ are excluded as per graviso 1: 138:175571 REFERENCE 138:95264 2: REFERENCE 138:69917 3: REFERENCE 137:329286 REFERENCE 4: 137:252731 REFERENCE 5:

REFERENCE 137:37406 7: REFERENCE 136:374545 8: REFERENCE 136:345763 9: REFERENCE

6:

136:196995 REFERENCE 10:

=> d ide can 123

L23 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 155955-25-2 REGISTRY

CN 4H-1-Benzopyran-4-one, 5-hydroxy-7-methyl-3-phenyl- (9CI) (CA

INDEX NAME)

FS 3D CONCORD

MF C16 H12 O3

SR CA

LC STN Files: CA, CAPLUS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 121:280544

=> s 140 not 142

L51 3 L40 NOT L42

=> d ide can tot

L51 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2003 ACS

RN 574-12-9 REGISTRY

CN 4H-1-Benzopyran-4-one, 3-phenyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Isoflavone (6CI, 7CI, 8CI)

OTHER NAMES:

CN 3-Phenylchromone

FS 3D CONCORD

MF - C15 H10 O2

CI COM

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CIN, CSCHEM, DDFU, DRUGU, EMBASE, HODOC\*, IFICDB, IFIPAT, IFIUDB, MRCK\*, NAPRALERT, PIRA, PROMT, SPECINFO, TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data)

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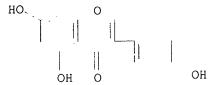
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423 REFERENCES IN FILE CA (1962 TO DATE)
               63 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
               425 REFERENCES IN FILE CAPLUS (1962 TO DATE)
               12 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
  REFERENCE
             1: 138:204203
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CN
     NAME)
OTHER CA INDEX NAMES:
CN Daidzein (6CI)
     Isoflavone, 4',7-dihydroxy- (8CI)
OTHER NAMES:
CN
    4',7-Dihydroxyisoflavone
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CN
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CN
CN
    Daidzeol
CN
    K 251b
CN
    NPI 031E
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      DRUGU, DRUGUPDATES, EMBASE, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA,
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        (*File contains numerically searchable property data)
    Other Sources: EINECS**
        (**Enter CHEMLIST File for up-to-date regulatory information)
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RTECS\*, SPECINFO, TOXCENTER, USPAT2, USPATFULL

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 (\*\*Enter CHEMLIST File for up-to-date regulatory information)



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REFERENCE 8: 138:231280

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=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 11:48:31 ON 15 APR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 15 Apr 2003 VOL 138 ISS 16 FILE LAST UPDATED: 14 Apr 2003 (20030414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L50 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2003 ACS
      2001:185742 HCAPLUS
      Preparation of isoflavones as therapeutic agents with estrogen
ΑN
DN
TΤ
      receptor binding activity
      Heaton, Andrew; Kumar, Naresh; Kelly, Graham
      Edmund; Husband, Alan
      Novogen Research Pty. Ltd., Australia
PΑ
      PCT Int. Appl., 44 pp.
SO
       CODEN: PIXXD2
       Patent
 DT
       English
       ICS C07D311-38; C07D471-06; C07C049-215; C07C049-213; A61K031-12;
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             A61P019-10; A61P019-02; A61P017-06; A61P007-00; A61P035-00;
             A61P025-28; A61P017-04; A61P001-00
       26-4 (Biomolecules and Their Synthetic Analogs)
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    GΙ
                                                                      OAc
                                  R4'
            R5
                                                       1
                                           Cl
                                  <sub>R</sub>3'
```

AcO

II

```
Isoflavanoids, such as I [R3', R4', R7 = H, OH, OAc, etc.; R5 = H, OH,
AΒ
    OAc, Me, etc.; R6 = H, Cl, etc.], were prepd. for pharmaceutical use in the treatment of diseases assocd. with estrogenic or androgenic
     effects. Thus, isoflavone II was prepd. in 75% yield by acetylation of
     6-chloro-7-hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one with acetic
     anhydride in pyridine. The prepd. isoflavanoids were tested for binding
     affinity for both subtypes of the estrogen receptor.
     isoflavanoid prepn estrogen receptor binding
ST
     Isoflavonoids
IT
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL
     (Biological study); RACT (Reactant or reagent); USES (Uses)
        (prepn. of isoflavones with estrogen receptor
        binding activity for pharmaceutical use)
     Estrogen receptors
TΤ
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
         (prepn. of isoflavones with estrogen receptor
        binding activity for pharmaceutical use)
                                                   328406-47-9P
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      (Reactant or reagent); USES (Uses)
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ΙT
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      328406-46-8P · 328406-48-0P
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      study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
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 TΤ
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (prepn. of isoflavones with estrogen receptor
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               THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE.CNT 14
 RE
 (1) Anticancer Inc; WO 9848790 A1 1998 HCAPLUS
 (2) Bannerjee; J Electrochem Soc India 1998, V47(4), P237 HCAPLUS
 (3) Children'S Hospital Oakland Research Institute; WO 9918953 A1 1999 HCAPLUS
 (4) Laboratoire L Lafon; WO 0003707 Al 2000 HCAPLUS
 (5) Lamberton; Aust J Chem 1978, V31(2), P455 HCAPLUS
 (6) Liepa; Aust J Chem 1981, V34(12), P2647 HCAPLUS
 (7) Lyonnaise Industrielle Pharmaceutique; FR 2693724 Al 1994 HCAPLUS
 (8) New Standard Gmbh; DE 4432947 Al 1996 HCAPLUS
 (9) Novogen Research Pty Ltd; WO 9808503 Al 1998 HCAPLUS
 (10) Novogen Research Pty Ltd; WO 9936050 Al 1999 HCAPLUS
 (11) Ota İsan Kk; JP 01226824 A 1989 HCAPLUS
 (12) Wahala; Heterocycles 1989, V28(1), P183 HCAPLUS
 (13) Weidenborner; Phytochemistry 1990, V29(3), P801
 (14) Zilliken; US 4157984 1979 HCAPLUS
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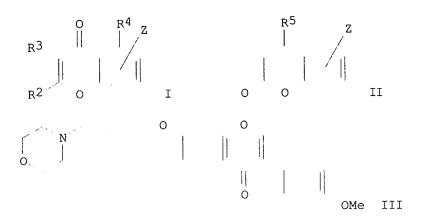
study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL

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RN
CN
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      Ме
      ANSWER 2 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 L50
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      Preparation of flavones, xanthones, and coumarins for pharmaceutical use
 ΑN
 DN
 ΤI
      in the treatment of cancer
      Bombardelli, Ezio; Valenti, Piero
 IN
       Indena S.p.A., Italy
 PΑ
       PCT Int. Appl., 46 pp.
 SO
       CODEN: PIXXD2
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       ICS C07D311-36; C07D311-16; C07D311-86; A61K031-37; A61P035-00
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MARPAT 134:207651

OS GI

328564-29-0P



AB Flavones, xanthones, and coumarins, such as I and II [Z = OCH2C.tplbond.CCH2NRR1; R, R1 = H, alkyl; NRR1 = nitrogen contg. heterocyclyl, such as 1-piperidinyl or 4-morpholinyl; R2, R3 = H, substituted aryl, such as hydroxyphenyl, etc.; R4 = H, OH, alkoxy, etc.; R5 = H, alkyl], were prepd. for pharmaceutical use as modulators of multiple drug resistance in cancer chemotherapy and for possible use in the treatment or prevention of other disorders, such as menopausal disorders and osteoporosis. Thus, isoflavone deriv. III was prepd. by reacting 7-hydroxy-4'-methoxyisoflavone with propargyl bromide using K2CO3 and KI in acetone to form 7-(2-propynyloxy)-4'-methoxyisoflavone, which was then reacted with formaldehyde and morpholine using CuSO4 in EtOH and H2O to form III. The prepd. compds. were tested for cytotoxicity against drug resistant breast cancer cells MDA-435/LCC6-MDR.

ST flavone xanthone coumarin prepn antitumor agent

IT Antitumor agents

(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in the treatment of cancer)

IT Flavonoids

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in

the treatment of cancer)
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(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in the treatment of cancer)

1T 90-33-5 106-96-7 109-89-7, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 123-75-1, Pyrrolidine, reactions 485-72-3 486-66-8 491-80-5 719-41-5 1915-98-6 2759-28-6

3722-51-8 6665-86-7 13004-42-7 **13057-72-2** 18651-15-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in the treatment of cancer)

The treatment of cancer;

67091-11-6P 67268-43-3P 124039-97-0P 328564-08-5P,

7-(2-Propynyloxy)-4'-methoxyisoflavone 328564-09-6P 328564-10-9P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in

the treatment of cancer) RE.CNT THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD RE (1) Allergan Inc; EP 0419132 A 1991 HCAPLUS (2) Allergan Inc; WO 9518803 A 1995 HCAPLUS (3) Francois, M; US 4151291 A 1979 HCAPLUS (4) Jay, P; US 3513198 A 1970 (5) Petrow, V; JOURNAL OF PHARMACY AND PHARMACOLOGY 1958, V10, P86 HCAPLUS ΤТ 486-66-8 13057-72-2 RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. of flavones, xanthones, and coumarins for pharmaceutical use in the treatment of cancer) RN 486-66-8 HCAPLUS 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX CN 0 OH RN 13057-72-2 HCAPLUS CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME) Ph L50 ANSWER 3 OF 19 HCAPLUS COPYRIGHT 2003 ACS 2000:756511 HCAPLUS ΑN DN 133:317571 TΙ Estrogen receptor -. beta. ligands for therapy Barlaam, Bernard Christophe; Piser, Timothy Martin PΑ Astrazeneca AB, Swed. SO PCT Int. Appl., 23 pp. CODEN: PIXXD2 DTPatent LA English IC ICM A61K031-00 CC 1-12 (Pharmacology) Section cross-reference(s): 27, 28 FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE \_\_\_\_ \_\_\_\_\_ PΙ WO 2000062765 A2 20001026 WO 2000-GB1380 20000411 <--WO 2000062765 20010907 А3 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

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     MARPAT 133:317571
OS
     receptor (ER) - . beta. comprises the step of administering a
AΒ
     therapeutically effective amt. of estrogen receptor
     -.beta.-selective ligands, which mimic estrogen replacement
     therapy (ERT), but lack undesirable side effects of ERT. The ligand
     satisfies the equation: (Ki.alpha.A/Ki.beta.A)/(Ki.alpha.E/Ki.beta.E) > 1,
     where Ki.alpha.A and Ki.beta.A are the Ki values for the agonists in
     ER-.alpha. and ER-.beta., and Ki.alpha.E and Ki.beta.E are the Ki values
     for estrogens in ER-.alpha. and ER-.beta., resp. Diseases
      assocd. with the ER-.beta. are Alzheimer's disease, anxiety, depression,
      osteoporosis, cardiovascular disease, rheumatoid arthritis, and prostate
      cancer. For example, (3-bromo-4-hydroxyphenyl)-5,7-dihydroxy-5H-1-
      benzopyran-4-one was prepd. using 1,3,5-trihydroxybenzaldehyde and
      3-bromo-4-hydroxyphenylacetic acid as starting compds.
      estrogen receptor ligand Alzheimer disease;
      antidepressant anxiolytic estrogen receptor ligand;
 ST
      antirheumatic estrogen receptor ligand; osteoporosis
      cardiovascular disease estrogen receptor ligand;
      prostate cancer estrogen receptor ligand
      Anti-Alzheimer's agents
 IT
      Antidepressants
      Antirheumatic agents
       Anxiolytics
          (estrogen receptor-.beta. ligands for treatment of
       Cardiovascular agents
          cardiovascular and neurol. disorders, rheumatoid arthritis,
          osteoporosis and prostate cancer)
       Estrogens
  ΤT
       RL: BAC (Biological activity or effector, except adverse); BSU (Biological
       study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
       BIOL (Biological study); PREP (Preparation); USES (Uses)
           (estrogen receptor-.beta. ligands for treatment of
          cardiovascular and neurol. disorders, rheumatoid arthritis,
          osteoporosis and prostate cancer)
        Hormone replacement therapy
           (mimicking; estrogen receptor-.beta. ligands for
  ΙT
           treatment of cardiovascular and neurol. disorders, rheumatoid
           arthritis, osteoporosis and prostate cancer)
        Prostate gland
   IT
           (neoplasm, inhibitors; estrogen receptor-.beta.
        Prostate gland
           ligands for treatment of cardiovascular and neurol. disorders,
           rheumatoid arthritis, osteoporosis and prostate cancer)
            (prostate gland; estrogen receptor-.beta. ligands
        Antitumor agents
   IT
            for treatment of cardiovascular and neurol. disorders, rheumatoid
            arthritis, osteoporosis and prostate cancer)
         Osteoporosis
            (therapeutic agents; estrogen receptor-.beta.
    IT
```

ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL Estrogen receptors TΤ (Biological study); PROC (Process) (.beta.; estrogen receptor-.beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) 6468-98-0P 5217-90-3P 6468-36-6P 5217-89-0P 480-23**-**9P 552-59-0P IT 18651-39-3P 18651-11-1P 15584-09-5P 15584-08-4P 13111-57-4P 36190-95-1P 31913-52-7P 24051-97-6P 24051-96-5P 21554-71-2P 63046-09-3P 62845-09-4P **62845-21-0P** 40624-03-1P 94105-90-5P 91805-21-9P 67295-48-1P **70943-68-9P** 101068-34-2P 101068-31-9P 96462-61-2P **96657-99-7P** 303012-54-6P 299951-78-3P 215435-34-0P 157405-88-4P 123731-49-7P 303012-59-1P 303012-58-0P 303012-57-9P 303012-56-8P 303012-55-7P 303012-64-8P 303012-63-7P 303012-62-6P 303012-61-5P 303012-60-4P 303012-67-1P 303012-66-0P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (estrogen receptor . beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) 156-38-7, 4-Hydroxyphenylacetic acid 487-70-7, 38692-80-7, 3-Bromo-4-hydroxyphenylacetic IT 2,4,6-Trihydroxybenzaldehyde acid RL: RCT (Reactant); RACT (Reactant or reagent) (estrogen receptor -. beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT 303012-69-3P IT (Reactant or reagent) (estrogen receptor-.beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) 62845-21-0P 70943-68-9P 96657-99-7P RL: BAC (Biological activity or effector, except adverse); BSU (Biological IT study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (estrogen receptor-.beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) 62845-21-0 HCAPLUS 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-5-methyl- (9CI) (CA RN CN INDEX NAME) OH

RN 70943-68-9 HCAPLUS CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)

Me

```
HO.
                  OH
RN
     96657-99-7 HCAPLUS
     4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(3-hydroxyphenyl)- (9CI) (CA INDEX
CN
     NAME)
HO.
           0
                       OH
      OH
    ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2003 ACS
     1999:597471 HCAPLUS
AN
     131:199621
DN
TI
     Multi-step preparation of high-purity ipriflavone
ΙN
     Ferrari, Massimo
PΑ
     Erregierre S.p.A., Italy
SO
     Eur. Pat. Appl., 10 pp.
     CODEN: EPXXDW
DT
     Patent
LA
     English
IC
     ICM C07D311-36
     ICS A61K031-35
     27-14 (Heterocyclic Compounds (One Hetero Atom))
     Section cross-reference(s): 26, 63
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                            DATE
PΙ
     EP 941992
                      A1
                            19990915
                                           EP 1999-103494
                                                            19990223 <--
     EP 941992
                      В1
                            20020508
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     IT 1298619
                      В1
                            20000112
                                           IT 1998-MI483
                                                            19980310 <--
     US 5973169
                            19991026
                                           US 1999-255043
                                                            19990222 <--
     JP 11292869
                       Α2
                            19991026
                                           JP 1999-60451
                                                            19990308 <--
PRAI IT 1998-MI483
                            19980310 <--
                       Α
OS
    CASREACT 131:199621
AΒ
     Ipriflavone, a calcium regulator used in the treatment of osteoporosis (no
     data), is prepd. in high yield and selectivity by: (A) the
     cyclocondensation of 2,4-dihydroxyphenyl benzyl ketone (I) with Et
     orthoformate in DMF at 115-120.degree. using a I wt./solvent vol. (w/v)
     ratio of <1/4 and in the presence of morpholine as a catalyst to yield
     7-hydroxyisoflavone (II); (B) sepn. of II from the reaction residue by its
     pptn. as its corresponding dicyclohexylamine salt, followed by
     neutralization with orthophosphoric acid to yield II; and (C)
     etherification of II with an iso-Pr halide (e.g., iso-Pr bromide) to give
     ipriflavone contg. .ltoreq.0.1% impurity.
ST
     ipriflavone manuf high purity; cyclocondensation manuf high purity
     ipriflavone; etherification manuf high purity ipriflavone
ΙT
     Precipitation (chemical)
        (of 7-hydroxyisoflavone dicyclohexylamine salt in the prepn. of
```

```
high-purity ipriflavone)
IT
     Etherification
        (of 7-hydroxyisoflavone with iso-Pr bromide in the manuf. of
        high-purity ipriflavone)
IT
     Cyclocondensation reaction
        (of benzyl 2,4-dihydroxyphenyl ketone with Et orthoformate in the
        prepn. of 7-hydroxyisoflavone)
ΙT
     110-91-8, Morpholine, uses
     RL: CAT (Catalyst use); USES (Uses)
        (multi-step prepn. of high-purity ipriflavone)
IT
     13057-72-2P, 7-Hydroxyisoflavone 241804-59-1P
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
    preparation); PREP (Preparation); RACT (Reactant or reagent)
        (multi-step prepn. of high-purity ipriflavone)
ΙT
     35212-22-7P, Ipriflavone
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (multi-step prepn. of high-purity ipriflavone)
IT
     75-26-3, Isopropyl bromide
                                  101-83-7, Dicyclohexylamine
                                                                 7664-38-2,
    Orthophosphoric acid, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (multi-step prepn. of high-purity ipriflavone)
ΙT
     122-51-0, Ethyl orthoformate
                                   3669-41-8, 2,4-Dihydroxyphenyl benzyl
     ketone
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (multi-step prepn. of high-purity ipriflavone from)
                     78-83-1, Isobutyl alcohol, uses
ΤТ
     68-12-2, uses
                                                      108-88-3, Toluene, uses
     7732-18-5, Water, uses
    RL: NUU (Other use, unclassified); USES (Uses)
        (solvent; multi-step prepn. of high-purity ipriflavone)
RE.CNT
              THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; WO 15 1991 HCAPLUS
(2) Chinoin; WO 9115483 A 1991 HCAPLUS
(3) Szerves Vegyipari Fejleszto Kosos Vallalat; HU 55376 A HCAPLUS
    13057-72-2P, 7-Hydroxyisoflavone 241804-59-1P
    RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
    preparation); PREP (Preparation); RACT (Reactant or reagent)
        (multi-step prepn. of high-purity ipriflavone)
RN
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
CN
          O.
                Ph
RN
    241804-59-1 HCAPLUS
```

4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl-, compd. with

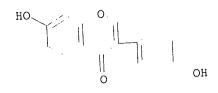
N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1 CRN 13057-72-2 CMF C15 H10 O3

CN

```
L50 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2003 ACS
AN
     1997:113419 HCAPLUS
     126:122303
DN
     Hair growth promoting compositions containing isoflavanoid derivatives
TΙ
     Kung, Patrick C.; Li, Ze Zeng
ΙN
     Kung, Patrick, C., USA
PΑ
     PCT Int. Appl., 20 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
IC
     ICM A01N043-16
     ICS A61K031-35
     62-3 (Essential Oils and Cosmetics)
     Section cross-reference(s): 1, 26, 63
FAN.CNT 1
                      KIND DATE
                                           APPLICATION NO.
     PATENT NO.
     ______
     WO 9639832
                     A1
                            19961219
                                          WO 1996-US8433
                                                            19960603 <--
PΙ
         W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IL,
             IS, JP, KG, KP, KR, KZ, LK, LR, LS, LT, LV, MD, MG, MK, MN, MX,
             NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, UZ, VN, AM,
             AZ, BY
         RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
             IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML,
             MR, NE, SN, TD, TG
                                           US 1995-484097
                                                            19950607 <--
                            19970617
     US 5639785
                      A
                                           AU 1996-59704
                                                            19960603 <--
     AU 9659704
                            19961230
                       A1
PRAI US 1995-484097
                            19950607
                                     <--
     US 1996-659466
                            19960531
                                      <--
     WO 1996-US8433
                            19960603
                                     <--
OS
     MARPAT 126:122303
     Novel compns. of isoflavanoid derivs. useful for the treatment of male
     pattern baldness and alopecia areata, promoting the conversion of gray
     hair to the original pigment in hair follicles, and increasing the blood
     supply to the brain are disclosed. The invention also relates to methods
     for treatment of male pattern baldness and alopecia areata, gray hair, and
     brain circulatory deficiencies. Sodium methoxide 6.48 was added to 50 mL
     DMF and the mixt. was distd. to eliminate alc. then, resulting product was
     cooled to .ltoreq.20.degree.. Dimethylamino-methoxy sulfuric acid Me
     ester (prepn. given) was added dropwise to the cooled product and the
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mixt. was allowed to react for 5 h. The reaction mixt. was distd. to
    remove dimethyllformaide from the mixt. followed by addn. of water to
    obtain daidzein (I). A tablet contained I 100, lactose 50, starch 23,
    microcryst. cellulose 2, dicalcium phosphate 30 mg, surfactants trace, and
    magnesium trace. The efficacy of tablets (2 tablet 3 times/day) in
    treatment of hypertensive male bald subject is reported.
    hair growth promoter isoflavanoid deriv; pharmaceutical tablet daidzein
    male baldness
       (areata; hair growth promoting compns. contg. isoflavanoid derivs.)
    Alopecia
        (cerebrovascular; hair growth promoting compns. contg. isoflavanoid
    Brain, disease
        derivs.)
     RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU
IT
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (growth stimulants; hair growth promoting compns. contg. isoflavanoid
     (Uses)
        derivs.)
     Isoflavonoids
     RL: RCT (Reactant); RACT (Reactant or reagent)
ΙT
         (hair growth promoting compns. contg. isoflavanoid derivs.)
        (male pattern; hair growth promoting compns. contg. isoflavanoid
     Alopecia
IT
         derivs.)
         (ointments, creams; hair growth promoting compns. contg. isoflavanoid
      Drug delivery systems
 ΙT
         derivs.)
         (ointments; hair growth promoting compns. contg. isoflavanoid derivs.)
      Drug delivery systems
 IT
         (tablets; hair growth promoting compns. contg. isoflavanoid derivs.)
      Drug delivery systems
 IT
                486-63-5P 486-66-8P, Daidzein 19725-36-1P
                                              142574-14-9P
      485-72-3P
                               139256-06-7P
 ΙT
      56401-04-8P 89019-85-2P
      146307-82-6P 148356-24-5P 186246-60-6P
                                               186246-61-7P
                                               186246-65-1P
      186246-62-8P 186246-63-9P 186246-64-0P
                                                  186246-69-5P
      RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU
                                    186246-68-4P
       (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
          (hair growth promoting compns. contg. isoflavanoid derivs.)
       (Uses)
                           75-93-4, Methyl sulfate
       68-12-2, reactions
       RL: RCT (Reactant); RACT (Reactant or reagent)
  TΤ
          (hair growth promoting compns. contg. isoflavanoid derivs.)
       486-66-8P, Daidzein 19725-36-1P 89019-85-2P
       148356-24-5P 186246-60-6P 186246-63-9P
  IT
       RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU
       (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
           (hair growth promoting compns. contg. isoflavanoid derivs.)
        (Uses)
        4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX
       486-66-8 HCAPLUS
  RN
  CN
        NAME)
```



ST

ΙT

IT

19725-36-1 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-(2-hydroxyphenyl)- (9CI) (CA INDEX CN NAME)

89019-85-2 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-(3-hydroxyphenyl)- (9CI) (CA INDEX CN

148356-24-5 HCAPLUS RN

4H-1-Benzopyran-4-one, 5-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX CN NAME)

186246-60-6 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-(acetyloxy)-3-(4-hydroxyphenyl)- (9CI) (CA INDEX CN NAME)

186246-63-9 HCAPLUS

4H-1-Benzopyran-4-one, 5-(acetyloxy)-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RNCN NAME)

186246-64-0 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-(acetyloxy)-3-(3-hydroxyphenyl)- (9CI) (CA INDEX CN

L50 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2003 ACS

1993:575863 HCAPLUS ΑN

DN

Isoflavones from soybean exudates inducing nodulation of Bradyrhizobium TIjaponicum.

Kosslak, Renee; Bookland, Roger; Appelbaum, Edward R. ΙN

Lubrizol Genetics, Inc., USA

PAU.S., 15 pp. Cont. of U.S. Ser. No. 35,516, abandoned. SO CODEN: USXXAM

DΤ Patent

English LA

ICM A01N063-00 ICS A01N043-00; C12R001-41; C12N001-00; C05F011-08; A01C001-06 IC

NCL 424-93A

5-2 (Agrochemical Bioregulators) CC Section cross-reference(s): 3, 10, 11

FAN.CNT 1

APPLICATION NO. DATE PATENT NO. KIND DATE \_\_\_\_\_ \_\_\_\_\_ \_\_\_\_\_ US 1989-393081 19890809 <--19930720 US 5229113 A

19870407 <--

PRAI US 1987-35516 The isoflavones daidzein and genistein of soybean exudates are identified as inducers of nodulation of Bradyrhizobium. These compds. can be used for regulated induction of nodulation or for expression of heterologous genes under expression of the nodulation promoter. Several other flavonoids are also identified as inducers, with daidzein and genistein effective at .ltoreq.1.mu.M. The compds. were identified by chromatog. fractionation of exudates and assaying fractions for induction of expression of a reporter gene from the nod promoter.

Bradyrhizobium nodulation inducer flavone soybean ST

Bradyrhizobium japonicum IT

(nodulation by, induction of, flavones from soybean exudates for)

Flavonoids ΙT

RL: BIOL (Biological study)

(nodulation inducers, by Bradyrhizobium japonicum, induction of nodABC genes by)

IT Soybean

(nodulation inoculum for, Bradyrhizobium japonicum and nodulation-inducing flavones in)

Flavonoids ΙT

RL: BIOL (Biological study)
(iso-, oxo, nodulation inducers, by Bradyrhizobium japonicum, induction of nodABC genes by)

IT Operon

(nodABCIJ, induction of, flavones for)

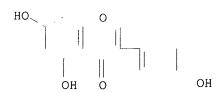
IT 446-72-0, Genistein 479-13-0, Coumestrol 485-72-3, Formononetin 486-66-8, Daidzein 491-80-5, Biochanin A 520-18-3, Kaempferol 520-36-5, Apigenin 2196-14-7 4044-00-2, 5,7-Dihydroxyisoflavone 13057-72-2, 7-Hydroxyisoflavone RL: BIOL (Biological study) (nodulation inducer, by Bradyrhizobium japonicum, induction of nodABC

(nodulation inducer, by Bradyrhizobium japonicum, induction of nodABC genes by)
-72-0. Genistein 486-66-8. Daidzein 4044-00-2

IT 446-72-0, Genistein 486-66-8, Daidzein 4044-00-2
, 5,7-Dihydroxyisoflavone 13057-72-2, 7-Hydroxyisoflavone
RL: BIOL (Biological study)
 (nodulation inducer, by Bradyrhizobium japonicum, induction of nodABC genes by)

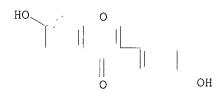
RN 446-72-0 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 486-66-8 HCAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 4044-00-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-phenyl- (9CI) (CA INDEX NAME)

RN 13057-72-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)

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HO. O Ph
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ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2003 ACS
    1993:535006 HCAPLUS
    119:135006
DN
    Carbon dioxide detector
TI
    Mills, Andrew; Chang, Qing
ΙN
    Johnson and Johnson Professional Products Ltd., UK
PΑ
     PCT Int. Appl., 19 pp.
SO
    CODEN: PIXXD2
     Patent
DT
     English
LA
     ICM G01N031-22
TC
     9-1 (Biochemical Methods)
CC
FAN.CNT 1
                                          APPLICATION NO. DATE
                     KIND DATE
     PATENT NO.
                           _____
                     ____
     _____
                                                           19930111 <--
                                          WO 1993-GB49
     WO 9314399
                            19930722
                      A1
PΙ
         W: JP, US
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
                                                           19930111 <--
                                           EP 1993-901829
                      A1 19941026
     EP 620918
                           19970730
                       В1
     EP 620918
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
                                                           19930111 <--
                                          JP 1993-512258
                     Т2
                            19950323
     JP 07502817
                            20010625
                       В2
     JP 3178839
                                                            19930111 <--
                                           AT 1993-901829
                            19970815
                       Ε
     AT 156269
                                                            19930111 <--
                                           ES 1993-901829
                       Т3
                            19971016
     ES 2105211
                                                            19940928 <--
                                           US 1994-256468
                       Α
                            19960102
     US 5480611
                            19920109 <--
PRAI GB 1992-431
                       Α
                                     <--
                            19930111
     WO 1993-GB49
                       W
     A CO2 detector comprises an indicating member and a CO2 sensing medium and
AΒ
     is useful for medical uses, esp. trachea intubation. The indicating
     member comprises an intimate mixt. of a polymer vehicle (polyvinyl
     butyral, polyvinyl Me ether, etc.). The CO2 sensing medium comprises an
     anionic fluorimetric dye (1,3-dihydroxypyrene-6,8-disulfonate,
     fluorescein, etc.) and a lipophilic org. quaternary cation
      (benzyltrimethylammonium, trioctylmethylammonium, etc.). Thus, a film
     contg. 1-hydroxypyrene-3,6,8-trisulfonate, tetraoctylammonium, Et
      cellulose, and tris-Bu phosphate was coated on the surface of a gas
      impermeable tube. Exposure of the film to a high level of CO2 converted
      the deprotonated form of the dye into its protonated form, which can be
      monitored by measuring at 394nm.
      carbon dioxide detector fluorescent film; dye fluorescent carbon dioxide
 ST
      detector
      Polymers, uses
 ΙT
      RL: USES (Uses)
         (indicating membrane contg., in carbon dioxide detector)
      Vinvl acetal polymers
 IT
      RL: USES (Uses)
         (butyrals, indicating membrane contg., in carbon dioxide detector)
 ΙT
         (fluorescent, anionic, sensing medium contg., in carbon dioxide
         detector for medical use)
 ΙT
      Sensors
          (gas, for carbon dioxide, for medical use)
```

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124-38-9, Carbon dioxide, analysis
ΤT
     RL: ANST (Analytical study)
         (detector for)
                605-45-8, Diisopropyl phthalate 56-81-5, Glycerine, uses
ΙT
     122-62-3
     70-55-3, p-Toluene sulphonamide 77-99-6, Trimethylolpropane 78-40-0,
     Triethyl phosphate
                           78-51-3
     RL: ANST (Analytical study)
        (in indicating membrane manuf. for carbon dioxide detector) 2-89-5, Poly(vinyl alcohol) 9003-09-2, Poly(vinyl methyl ether)
     9002-89-5, Poly(vinyl alcohol) 9003-09-2, Poly(vinyl methy 9003-53-6, Polystyrene 9004-32-4, Carboxymethyl cellulose
IT
     Ethylcellulose
                       9004-64-2, Hydroxypropyl cellulose
                                                             9004-67-5,
                      9011-14-7, Poly(methyl methacrylate)
     Methylcellulose
                                                                  25322-68-3,
     Polyethylene glycol
                             25322-69-4, Polypropylene glycol
                                                                  126-73-8,
     Tributyl phosphate, uses
     RL: ANST (Analytical study)
         (indicating membrane contg., in carbon dioxide detector)
ΙT
     84-87-7, 1-Naphthol-4-sulfonic acid
                                              90-33-5
                                                         93-01-6,
                                    93-35-6, Umbelliferone
     2-Naphthol-6-sulfonic acid
                                                               567-18-0,
                                    583-17-5, 2-Hydroxycinnamic acid
                                                                         779-27-1,
     1-Naphthol-2-sulfonic acid
     7-Hydroxycoumarin-3-carboxylic acid 1214-24-0, 3,6-DiHydroxyxanthone
     2321-07-5, Fluorescein 3030-97-5, Salicylaldehyde semicarbazone 3722-51-8, 3-Hydroxyxanthone 6665-86-7, 7-Hydroxyflavone
     13057-72-2, 7-Hydroxyisoflavone 15463-09-9, 7-Hydroxylepidine
     20168-55-2, 3-Hydroxyacridone 27928-00-3 58851-99-3 85353-28-2
     85644-14-0
     RL: ANST (Analytical study)
         (sensing medium contg. fluorescent, in carbon dioxide detector)
                  10549-76-5, Tetrabutylammonium 14800-24-9,
TI
     Benzyltrimethylammonium 18198-39-5, Tetraphenylphosphonium 19524-73-3,
                           20256-54-6, Tetrahexylammonium 22061-11-6
     Tetraoctylammonium
                   66997-36-2
     45306-06-7
     RL: ANST (Analytical study)
         (sensing medium contg., in carbon dioxide detector)
     13057-72-2, 7-Hydroxyisoflavone
TT
     RL: ANST (Analytical study)
         (sensing medium contg. fluorescent, in carbon dioxide detector)
RN
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
CN
           0
    Ph
L50 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2003 ACS
     1993:185706 HCAPLUS
ΑN
DN
     118:185706
     Method using daidzin or daidzin analog for the inhibition of aldehyde
TΙ
     dehydrogenase I (ALDH-I), and use in the treatment of alcohol dependence
     or alcohol abuse
IN
     Vallee, Bert L.; Keung, Wing Ming
     Endowment for Research in Human Biology, Inc., USA
PΑ
     PCT Int. Appl., 98 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
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IC

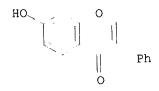
ICM A61K031-35

ICS C07D311-36; A61K031-70

4-7 (Toxicology) CC Section cross-reference(s): 7, 11, 27, 63 FAN.CNT 2 APPLICATION NO. DATE KIND DATE PATENT NO. -----\_\_\_\_ 19920630 <--19930121 WO 1992-US5598 WO 9300896 Α1 PΙ W: AU, BR, CA, FI, HU, JP, KR, NO, RO, RU, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE 19910701 <--US 1991-723404 19930420 US 5204369 Α 19920630 <--AU 1992-23085 19930211 AU 9223085 A1 19920630 <--EP 1992-915216 19940420 Α1 EP 592583 20010131 В1 EP 592583 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE AT 1992-915216 19920630 <--E 20010215 AT 198983 19920630 <--JP 1993-502339 20010528 В2 JP 3170281 19931230 <--NO 1993-4911 19940228 Α NO 9304911 19940524 <--US 1994-170272 19970429 A US 5624910 US 1998-190360 19981112 <--В1 20010703 US 6255497 A2 19910701 <--PRAI US 1991-723404 19920630 <--WO 1992-US5598 Α A1 19940524 <--US 1994-170272 19970429 <--А3 US 1997-840360 MARPAT 118:185706 OS ALDH-I is inhibited by daidzin (I) or an analog thereof, optionally with AΒ factor(s) increasing the bioavailability of the I or I analog. Such inhibitory compds. or compns. are useful as pharmaceutical compns in methods for the treatment of alc. dependence (i.e. alcoholism) or alc. abuse, for alc. sensitization, for extinguishing an alc.-drinking response, for suppressing an urge for alc., for inducing alc. intolerance, for preventing alcoholism in an individual with or without a susceptibility or predisposition to alc. or alc. abuse, and for limiting alc. consumption in an individual, whether or not the individual is genetically predisposed. I was isolated from the crude drug Radix Puerariae (prepd. as the dried root of Pueraria lobata). Kinetic consts. for the inhibition by I of ALDH isoenzymes I and II were 40 and 20,000 nM, resp. Prepn. and inhibitory activity of ether derivs., e.g. daidzein 7-(.omega.-carboxydecyl) ether, is also presented. I, at doses of 5, 10, and 30 mg/day suppressed alc. intake by hamsters by 20, 50, and 80%, resp. I in a crude Radix Puerariae methanolic ext. was 5-10 times more potent than pure I. daidzin aldehyde dehydrogenase inhibitor; alcoholism treatment daidzin ST Drug bioavailability IΤ Solubility (daidzen compn. including factor increasing) Molecular structure-biological activity relationship ΙT (of aldehyde dehydrogenase I isoenzymes inhibition by daidzin and related compds.) Kinetics, enzymic IT(of aldehyde dehydrogenase I isoenzymes inhibition by daidzin and related compds., inhibition consts. for) Drug dependence ΙT (alcoholism, treatment of, daidzin for, aldehyde dehydrogenase I inhibition in relation to) Kudzu IT (P. lobata, daidzin from Radix Puerariae of, aldehyde dehydrogenase I inhibition by, alcoholism treatment in relation to) IT Kudzu (P. lobata, roots, daidzin from, aldehyde dehydrogenase I inhibition by, alcoholism treatment in relation to) 486-66-8D, analogs 552-66-9, Daidzin ΙT RL: BIOL (Biological study) (aldehyde dehydrogenase I inhibition with, alcoholism treatment in

relation to)

```
529-59-9,
                                             525-82-6, Flavone
                          486-62-4, Ononin
     480-44-4, Acacetin
                552-59-0, Prunetin 2555-30-8, 7-Hydroxy-4-phenylcoumarin
IT
     Genistin
                                           146699-00-5 146699-01-6
                               88407-29-8
                  36136-92-2
     13057-72-2
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     study, unclassified); BIOL (Biological study)
        (aldehyde dehydrogenase inhibitory activity of)
     9003-39-8, Polyvinylpyrrolidone 11024-24-1, Digitonin 25322-68-3, PEG
ΙT
     RL: BIOL (Biological study)
        (daidzin soly. with)
     7585-39-9, .beta.-Cyclodextrin
ΙT
     RL: BIOL (Biological study)
     (daidzin soly. with PEG and) 64-17-5, Ethanol, biological studies
ΙT
     RL: BIOL (Biological study)
        (intolerance to, induction of, daidzin for, aldehyde dehydrogenase I
        inhibition in relation to)
     9028-86-8, Aldehyde dehydrogenase
ΙT
     RL: BIOL (Biological study)
        (isoenzyme I, inhibition of, by daidzin or daidzin analog, alcoholism
        treatment in relation to)
                                                  146698-99-9P
                                    146698-98-8P
                   146698-97-7P
     146698-96-6P
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and aldehyde dehydrogenase I inhibitory activity of)
                                   147158-76-7P
     147158-74-5P 147158-75-6P
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     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of)
                              2834-05-1, .omega.-Bromoundecanoic acid
      75-03-6, Ethyl iodide
      4224-70-8, .omega.-Bromohexanoic acid 30515-28-7, .omega.-Bromoheptanoic
ΙT
      acid
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with daidzin)
      486-66-8D, analogs
 ΙT
      RL: BIOL (Biological study)
         (aldehyde dehydrogenase I inhibition with, alcoholism treatment in
         relation to)
      4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX
 RN
 CN
      NAME)
 HO.
                         OH
      RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 ΙT
      study, unclassified); BIOL (Biological study)
          (aldehyde dehydrogenase inhibitory activity of)
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       4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
  RN
  CN
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ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2003 ACS
L50
ΑN
     1992:591584 HCAPLUS
DN
     117:191584
     An improved process for the preparation of substituted isoflavone
TI
     derivatives
     Kallay, Tamas; Lanyi, Gyorgy; Ledniczky, Laszlo; Emrei, Lajos; Hoffmann,
IN
     Gyorgy; Sziladi, Maria; Somfai, Eva; Montay, Tibor
     Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt., Hung.
PA
SO
     PCT Int. Appl., 22 pp.
     CODEN: PIXXD2
DΨ
     Patent
LA
     English
     ICM C07D311-36
IC
ICA
    A61K031-35
     26-4 (Biomolecules and Their Synthetic Analogs)
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     PATENT NO.
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                             DATE
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                                                              DATE
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                             19911017
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     WO 1990-HU23
                             19900406
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     CASREACT 117:191584; MARPAT 117:191584
OS
GΙ
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AB Isoflavones I (R = H, CHMe2; R1, R2 = H, OMe, OEt) were prepd. by cyclizing 2,4-(HO)2C6H3COCH2C6H3R1R2 with HC(OEt)3 in the presence of base and, optionally alkylating I(R = H). Thus, 2,4-(HO)2C6H3COCH2Ph was treated with HC(OEt)3 and morpholine in HOCHMe2 to give 90.6% I (R-R2 = H) contg. 0.2-0.4% I (R = Et, R1, R2 = H).

ST hydroxyphenylacetophenone cyclization orthoformate; hydroxyisoflavone; isoflavone hydroxy

IT Cyclocondensation reaction

(of dihydroxyphenyl benzyl ketones with orthoformate, isoflavones by)

IT 122-51-0, Triethylorthoformate

RL: RCT (Reactant); RACT (Reactant or reagent) (cyclization of, with dihydroxyphenyl benzyl ketones)

```
138948-69-3
                 24126-98-5
ΙT
     3669-41-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclization of, with orthoformate)
     138948-68-2P
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and alkylation of)
                                                       35212-22-7P,
                                         24160-14-3P
     13057-72-2P, 7-Hydroxyisoflavone
ΙT
     7-Isopropoxyisoflavone 138948-70-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
     138948-68-2P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and alkylation of)
     138948-68-2 HCAPLUS
RN
     Carbonic acid, monopotassium salt, compd. with 7-hydroxy-3-phenyl-4H-1-
CN
     benzopyran-4-one potassium salt (1:1) (9CI) (CA INDEX NAME)
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          79130-53-3
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      CMF C H2 O3 . K
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 HO-C-OH
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      13057-72-2P, 7-Hydroxyisoflavone
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      RL: SPN (Synthetic preparation); PREP (Preparation)
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      13057-72-2 HCAPLUS
      4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
 RN
 CN
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L50 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2003 ACS
     1988:549354 HCAPLUS
     Preparation and formulation of 3-aryl-3,4-dihydro-2H-1-benzopyrans useful
ΑN
DN
ΤI
     in treatment of vascular diseases
     Albert, Alban Imre; Zilliken, Friedrich W.
IN
     Zyma S. A., Switz.
PΑ
     Eur. Pat. Appl., 23 pp.
SO
     CODEN: EPXXDW
     Patent
DT
     English
LA
     ICS C07D493-04; C07D311-64; A61K031-35; A61K031-36
     ICM C07D311-58
IC
     27-14 (Heterocyclic Compounds (One Hetero Atom))
     Section cross-reference(s): 1
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HU 1987-4930 ZA 8708245 19890628 19871104 <--Α2 AU 1987-80655 HU 48611 19880505 A1 AU 8780655 19910131 19871104 <--В2 JP 1987-277528 AU 606087 19880602 19871104 <--Α2 JP 63130589 US 1987-116737 19890321 Α US 4814346 19861104 <--PRAI GB 1986-26344 MARPAT 109:149354 OS GΙ

Title compds. I [R = H, (un)substituted alkyl; one of R1 and R2 = H0, alkoxy, alkanoyloxy, alkyl and the other is H, or ORR1 = (un)substituted AΒ OCH20; R2 = H, or ORR2 = (un) substituted OCH20; B is (un) substituted by alkyl, phenylalkyl, alkanoyloxy, halo, amino, etc.] and their salts, useful for treatment of vascular diseases (no data) were prepd. 6,7-Dihydroxy-3-(3,4-dimethoxyphenyl)-4H-1-benzopyran-4-one in dioxane and

```
EtOH is hydrogenated for 8 days over Pd/C to give I [R, R2 = H, R1 = HO; B
     = 3,4-(Me20)2.
     aryldihydrobenzopyran prepn vascular disease treatment; benzopyran
ST
     aryldihydro prepn vascular disease
     Blood vessel, disease or disorder
TΤ
        (treatment of, aryldihydrobenzopyrans)
     Blood vessel, disease or disorder
        (Raynaud's phenomenon, treatment of, aryldihydrobenzopyrans for)
TT
     93-17-4, (3,4-Dimethoxyphenyl)acetonitrile
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (Friedel-Craft acylation of phenols by)
                                              459-22-3, (4-
     140-53-4, (4-Chlorophenyl)acetonitrile
IT
                                501-00-8, (3-Fluorophenyl)acetonitrile
     Fluorophenyl)acetonitrile
                                            622-75-3, 1,4-
     555-21-5, (4-Nitrophenyl)acetonitrile
                            1529-41-5, (3-Chlorophenyl)acetonitrile
     Benzenediacetonitrile
     2338-76-3, (3-Trifluoromethylphenyl)acetonitrile 2947-60-6,
                                    2947-61-7, 4-Methylphenylacetonitrile
     (3-Methylphenyl) acetonitrile
     4395-87-3, (4-Isopropylphenyl)acetonitrile
                                                  5689-33-8
                                                               13288-86-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (Friedel-Craft acylation with phenols)
                                       533-73-3, 1,2,4-Trihydroxybenzene
                           136-77-6
     87-66-1, Pyrogallol
ΙT
     608-25-3, 2,6-Dihydroxytoluene
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (Friedel-Crafts acylation with acetonitriles)
                 116743-80-7
     93434-89-0
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (cyclization of)
     3132-64-7, Epibromohydrin
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (cyclocondensation of, with hydroxybenzopyranone deriv.)
      94105-89-2
 IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (esterification by, of acetic anhydride)
                   97148-44-2
      76397-87-0
 ΙT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (esterification with, of acetic anhydride)
      3162-40-1
 ΙT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (etherification of, with Et bromobutyrate)
      533-68-6, Ethyl 2-bromobutyrate
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (etherification of, with hydroxyphenylbenzopyranone deriv.)
      2051-90-3, Dichlorodiphenylmethane
 ΙT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (etherification with, of dihydroxybenzopyran deriv.)
                                          37816-19-6 74693-73-5
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                  3162-32-1
      2746-87-4
 ΙT
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      75187-63-2
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (hydrogenation of)
                                                                   116718-45-7P
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          (prepn. and cyclization of)
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     (Reactant or reagent)
        (prepn. and hydrogenation of)
IΤ
     116719-30-3P
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     (Reactant or reagent)
        (prepn. and hydrolysis of)
     116718-52-6P
IT
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     (Reactant or reagent)
        (prepn. and reactions of)
                    116718-56-0P
ΙT
     116718-54-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, as intermediate for benzopyrans for treatment of vascular
        diseases)
ΙT
     116719-37-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, for treatment of muscular disease)
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        (prepn. of, for treatment of vascular disease)
     98-09-9, Benzenesulfonyl chloride
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (sulfonylation by, of aminophenylbenzopyranone deriv.)
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TΤ
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (hydrogenation of)
RN
     75187-63-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7,8-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX
CN
     NAME)
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English

LA

L50 ANSWER 11 OF 19 HCAPLUS COPYRIGHT 2003 ACS

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1988:523795 HCAPLUS
AN
     109:123795
DN
     Cloning and sequencing of Bradyrhizobium japonicum nodD gene, recombinant
ΤI
     Bradyrhizobium or Rhizobium containing the gene, and flavones for inducing
     expression of the gene
     Appelbaum, Edward R.; Hennecke, Hauke; Lamb, Joseph W.; Gottfert, Michael
ΙN
     Lubrizol Genetics, Inc., USA
PA
SO
     PCT Int. Appl., 90 pp.
     CODEN: PIXXD2
DT
     Patent
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ICM C12N015-00
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    ICS C12N005-00; C07H015-12; A01H001-04
     3-4 (Biochemical Genetics)
CC
     Section cross-reference(s): 10, 11
FAN.CNT 2
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                    KIND DATE
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                                                          19870617 <--
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PRAI US 1986-875297
                          19860617 <--
     The nodD genes of Bradyrhizobium japonicum are isolated and sequenced.
AΒ
     These gene and recombinant DNA mols. contg. them are useful for
     engineering Rhizobium and Bradyrhizobium strains exhibiting enhanced
     competitiveness for nodulation, and for selective manipulation of
     nodulation host range of these strains. The nodD gene of B. japonicum
     USDA123 was isolated by genomic DNA screening using hybridization probes.
     Clone pEA5-1B contained two nodD open reading frames, designated nodD-1
     and nodD-2. A HindIII fragment of the B. japonicum USDA123 contg. nodD,
     the promoter region of nodD and nodA, and the amino terminal end of nodC
     was joined to the lacZ gene through nodC to produce plasmids pEA2-21 and
     pEA4-10. The fusion gene was inducible by soybean exudates and compds.
     such as 7-hydroxyisoflavone in B. japonicum contg. either of the plasmids.
     nodD gene Bradyrhizobium sequence cloning; hydroxyflavone nodD gene
ST
     Bradyrhizobium induction
     Legume
ΤТ
     Soybean
        (exudates, induction of nodulation in recombinant Rhizobium or
        Bradyrhizobium contg. nodD gene with)
ΙT
     Root nodule
        (formation induction of, in recombinant Rhizobium or Bradyrhizobium
        contg. nodD gene)
IT
     Bradyrhizobium
     Rhizobium
         (nodulation gene promoter of, for nodD gene expression in recombinant
        Rhizobium or Bradyrhizobium)
     Molecular cloning
IT
         (of nodD genes of Bradyrhizobium japonicum, in Escherichia coli)
      Bradyrhizobium japonicum
TΤ
         (nodD gene of, cloning and sequencing of)
      Plasmid and Episome
 ΙT
         (pEA4-10, nodD-lacZ chimeric gene on, cloning and expression in
         Bradyrhizobium of)
      Plasmid and Episome
 IT
         (pRJ103, genes nodD1 and nodD2 of Bradyrhizobium japonicum on)
      Gene and Genetic element
 IT
      RL: BIOL (Biological study)
         (promoter, of nodulation gene of Rhizobium, for nodD gene expression in
         recombinant Rhizobium or Bradyrhizobium)
      Gene and Genetic element, microbial
 ΙT
      RL: BIOL (Biological study)
         (nodD, cloning and sequencing of, of Bradyrhizobium japonicum)
      Gene and Genetic element, microbial
 IΤ
      RL: BIOL (Biological study)
         (nodD1, cloning and sequencing of, of Bradyrhizobium japonicum)
      Gene and Genetic element, microbial
 ΙT
      RL: BIOL (Biological study)
         (nodD2, cloning and sequencing of, of Bradyrhizobium japonicum)
```

(nodABC, promoter of, of Bradyrhizobium japonicum, for nodD gene Operon IT expression in recombinant Rhizobium or Bradyrhizobium) 116412-15-8, Protein (Bradyrhizobium japonicum clone pEA5-1B gene nodD2 IT reduced) (amino acid sequence and cloning and expression of gene for) RL: PRP (Properties) 116412-14-7, Protein (Bradyrhizobiúm japonicum clone pEA5-1B gene nodD1 IT reduced) RL: PRP (Properties) (amino acid sequence and expression of gene for) 116411-89-3, Deoxyribonucleic acid (Bradyrhizobium japonicum clone pEA5-1B 116411-90-6, Deoxyribonucleic acid (Bradyrhizobium japonicum IT gene nodD1) clone pEA5-1B gene nodD2) RL: PRP (Properties) (cloning and expression and nucleotide sequence of) 116411-91-7, Deoxyribonucleic acid (Bradyrhizobium japonicum clone pEA5-1B gene nodD1 plus 5'- and 3'-flanking region fragment) 116411-92-8, ΙT Deoxyribonucleic acid (Bradyrhizobium japonicum clone pEA5-1B gene nodD2 plus 5'- and 3'-flanking region fragment) RL: PRP (Properties); BIOL (Biological study) (nucleotide sequence of) 446-72-0, Genistein 486-66-8, Daidzein IT RL: PRP (Properties) (nod gene induction with) 520-18-3, 491-80-5 485-72-3, Formononetin Kaempferol 520-36-5, Apigenin 552-59-0, Prunetin 4044-00-2, TT 5,7-Dihydroxyisoflavone 13057-72-2, 7-Hydroxyisoflavone (nodD gene induction with, in recombinant Bradyrhizobium or Rhizobium) RL: PRP (Properties) 446-72-0, Genistein 486-66-8, Daidzein TTRL: PRP (Properties) (nod gene induction with) 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RN CN NAME) OH OH4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RN CN

NAME)

4044-00-2, 5,7-Dihydroxyisoflavone 13057-72-2, IT

7-Hydroxyisoflavone

RL: PRP (Properties)

(nodD gene induction with, in recombinant Bradyrhizobium or Rhizobium)

RN 4044-00-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-phenyl- (9CI) (CA INDEX NAME)

RN 13057-72-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)

L50 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1986:5774 HCAPLUS

DN 104:5774

TI Benzopyran-4-one derivatives

IN Yamazaki, Iwao; Sawa, Yoichi

PA Takeda Chemical Industries, Ltd., Japan

SO Eur. Pat. Appl., 18 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM C07D311-36

ICS A61K031-35

CC 27-14 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 63

FAN.CNT 2

TIM, CNI Z													
	PAT	FENT :	NO.		KIND	DATE			API	PLICATION N	Ю.	DATE	
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ΡI	ΕP	1469	22		A2	19850	0703		EΡ	1984-11584	0	19841219	<
	EΡ	1469	22		A3	19860	0402						
	ΕP	1469	22		B1	1988	0907						
		R:	BE,	CH,	DE, FR	, GB,	IT,	LI,	NL, S	SE			
	JΡ	6013	2976		A2	19850	0716		JP	1983-24278	0	19831221	<
	HU	3713	8		0	1985	1128		HU	1984-4748		19841220	<
	US	4644	012		A	19870	0217		US	1984-68414	4	19841220	<
PRAI	JΡ	1983	-242	780		1983	1221	<	-				
	JΡ	1983	-242	779		1983	1221	<	_				
GI													

```
The title compds. I (R1 = H or OH; R2 = H or carboxyalkyl) prepd. by the
    reaction of I (R1 as above, R2 = H) with R3CHXCO2R4 (R3 = alkyl; R4 = H or
AΒ
    alkyl; X = halo) in presence of an inert solvent and a deacidifying agent
    followed by hydrolysis of the ester obtained, are bone resorption
    inhibitors, and as such are useful in osteoporosis treatment. Thus,
     7-hydroxy-3-phenyl-4H-1-benzopyran-4-one (I; R1 = R2 = H) was reacted with
     Et 2-bromopropionate in DMF in the presence of K2CO3 to give
     7-[[1-(ethoxycarbonyl)ethyl]oxy]-3-phenyl-4H-1-benzopyran-4-one which was
     hydrolyzed to 7-[(1-carboxyethyl)oxy]-3-phenyl-4H-1-benzopyran-4-one (I;
     R1 = H, R2 = MeCHCO2H) (II). II demonstrated its effectiveness as bone
     resorption inhibitor in rat fetal long bone culture. A tablet formulation
     contained II 200, lactose 15, starch 45, Ca CM-cellulose 10, and Mg
     stearate 1 g, for 1000 uncoated tablets 8.5\ \mathrm{mm} diam.
     phenylbenzopyranone prepn bone resorption inhibitor; carboxyalkylphenyl
ST
     benzopyranone prepn pharmaceutical; osteoporosis treatment
     carboxyalkylphenylbenzopyranone prepn
        (resorption of, inhibitors of, [(carboxyethyl)oxy]phenylbenzopyranones)
IΤ
     Osteoporosis
IT
        (treatment of, [(carboxyethyl)oxy]phenylbenzopyranones for)
                  99007-90-6P
     99007-87-1P
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and bone resorption-inhibiting activity of)
                                99007-85-9P
                                               99007-86-0P
                  99007-84-8P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     38594-18-2P
IT
      (Reactant or reagent)
         (prepn. and hydrolysis of)
     99007-88-2P
                    99007-89-3P
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, as bone resorption inhibitor)
     13057-72-2 19725-36-1 89019-85-2
 IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with Et bromopropionate)
      486-66-8
 IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with ethylbromopropionate)
      535-11-5
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with hydroxyphenylbenzopyranones)
      13057-72-2 19725-36-1 89019-85-2
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with Et bromopropionate)
      13057-72-2 HCAPLUS
      4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
 RN
 CN
                 Ph
      19725-36-1 HCAPLUS
      4H-1-Benzopyran-4-one, 7-hydroxy-3-(2-hydroxyphenyl)- (9CI) (CA INDEX
 RN
 CN
```

NAME)

89019-85-2 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-(3-hydroxyphenyl)- (9CI) (CA INDEX CN

ΙT 486-66-8

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with ethylbromopropionate)

RN 486-66-8 HCAPLUS

4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX CN

L50 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2003 ACS

1985:583568 HCAPLUS

DN 103:183568

Use of 3-phenyl-4H-1-benzopyran-4-one derivatives for inhibiting and TIΙN

Tsuda, Masao; Sawa, Yoichi; Yamazaki, Iwao PΑ

Takeda Chemical Industries, Ltd. , Japan SO

Ger. Offen., 17 pp. CODEN: GWXXBX

DΤ Patent

LΑ German

ΙC ICM A61K031-35

63-6 (Pharmaceuticals) CC

Section cross-reference(s): 1, 27

FAN	CNT 2	crerenc	e(s): 1, 27		
	PATENT NO.	KIND	DATE	APPLICATION NO.	DAMP
PI PRAI	DE 3446246 JP 60132917 EP 146921 EP 146921 R: BE, CH, US 4644012 JP 1983-242779	DE, FR, A	19850711 19850716 19850703 19860402 , GB, LI, NL, 19870217 19831221 <	DE 1984-3446246 JP 1983-242779 EP 1984-115839	

JP 1983-242780 CASREACT 103:183568 19831221 <---

OS GΙ

I (R = CO2H, group convertible to CO2H; R1, R2 = H, alkyl; R3 = H, OH) inhibit bone resorption. Pharmaceuticals contg. I are effective in the AΒ prevention and treatment of osteoporosis caused by decreased estrogen secretion after menopause in women. I suppressed the bone resorption by .apprx.5%. Acute toxicity studies with mice and rats showed no death incidence and toxic symptoms. Thus, tablets were prepd., each contg. 200 mg I (R = CO2H, R1 = Me, R2 = R3 = H)(II) [99007-90-6]. II was prepd. by hydrolysis of the Et ester [99007-84-8] which was prepd. from  $\frac{1}{2}$ 7-hydroxy-3-phenyl-4H-1-benzopyran-4-one [13057-72-2] and Et 2-bromopropionate [535-11-5].

phenylbenzopyranone drug osteoporosis ST

Osteoporosis ΙT

(treatment of, phenylbenzopyranone derivs. for)

99007-84-8P 99007-85-9P 99007-86-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT ΙT (Reactant or reagent)

(prepn. and hydrolysis of)

99007-90-6P 99007-88-2P 99007-89-3P 99007-87-1P IT

RL: PREP (Preparation)

(prepn. of, for treatment of osteoporosis)

486-66-8 13057-72-2 IT

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with Et bromopropionate)

ΙT

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with hydroxyphenylbenzopyranones)

486-66-8 13057-72-2 TT

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with Et bromopropionate)

4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RN CN NAME)

RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME) CN

```
ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2003 ACS
L50
    1985:437276 HCAPLUS
ΑN
    Isoflavones useful as anti-inflammatory agents
DN
TI
     Wu, Edwin S.
IN
     U.S., 4 pp. Cont.-in part of U.S. Ser. No. 259,403, abandoned.
     Pennwalt Corp. , USA
PA
SO
     CODEN: USXXAM
     Patent
DT
     English
LA
     ICM A61K031-35
IC
     ICS C07D311-36
     26-4 (Biomolecules and Their Synthetic Analogs)
NCL
     Section cross-reference(s): 1
                                          APPLICATION NO. DATE
 FAN.CNT 4
                     KIND DATE
      PATENT NO.
      _____
                                                          1.9821115 <--
                                          US 1982-441889
                                                          19821115 <--
                            19850226
                      Α
                                          US 1982-441890
      US 4501755
 PΙ
                            19850122
                                                          19860714 <--
                      A
                                          US 1986-885517
      US 4495198
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      US 1981-259387
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                            19811214
      US 1981-330122
                            19821115 <--
      US 1982-441893
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RR1NCH2CH (OH) CH2O. Ph

- Isoflavones I (R = H, alkyl, cycloalkyl; R1 = H, Me; R2 = H, alkyl, CF3, cycloalkyl, furyl) were prepd. Thus 7-hydroxy-3-phenylchromone was treated with epichlorohydrin, followed by aminolysis with H2NCHMe2 to give AΒ I (R = CHMe2, R1 = R2 = H) which at 50 mg/kg orally gave 45% inhibition in
- phenylchromonyloxypropanolamine prepn antiinflammatory; propanolamine phenylchromonyloxy; isoflavone aminohydroxypropoxy ST

Ι

Inflammation inhibitors and Antiarthritics IT

(isoflavonyloxypropanolamines)

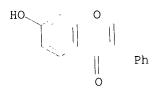
ΙT

GΙ

RL: RCT (Reactant); RACT (Reactant or reagent) (aminolysis of epoxypropoxyisoflavone by)

84858-46-8P 84858-48-0P 84858-64-0P 97124-31-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT IT

```
(Reactant or reagent)
        (prepn. and aminolysis of)
                 84858-24-2P 84858-47-9P 84858-49-1P 84858-50-4P
    84858-22-0P
ΙT
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. and antiinflammatory activity of)
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
ΙT
     (Reactant or reagent)
        (prepn. and quaternization of)
                                                             97124-34-0P
                                               97124-33-9P
                   84858-45-7P 97124-32-8P
     84858-44-6P
TT
     97138-90-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
                                                     97124-30-6
                                        84858-65-1
     2859-88-3 13057-72-2 32131-70-7
TT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with epichlorohydrin)
     106-89-8, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
TΤ
        (reaction of, with hydroxyisoflavone)
     13057-72-2
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with epichlorohydrin)
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
RN
CN
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L50 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2003 ACS
    1983:107161 HCAPLUS
ΑN
    98:107161
DN
    Antihypertensive agents
TI
    Wu, Edwin Shen Chou
IN
    Pennwalt Corp. , USA
PΑ
    Eur. Pat. Appl., 26 pp.
SO
    CODEN: EPXXDW
DΤ
    Patent
    English
LΑ
    C07D311-26; A61K031-35
IC
     27-14 (Heterocyclic Compounds (One Hetero Atom))
     Section cross-reference(s): 1, 63
FAN.CNT 4
                                      APPLICATION NO. DATE
     PATENT NO. KIND DATE
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                                      EP 1982-102950 19820406 <--
                   A1 19821110
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                    Al 19821104
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     FI 8201514
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                                                             19860714 <--
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     EP 1982-102950
                                       <--
                             19821115
     US 1982-441893
     CASREACT 98:107161
OS
GΙ
```

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Antihypertensive chromones I (R = H, alkyl, cycloalkyl; R1 = H, alkyl, F3C, Ph, o-ClC6H4, p-ClC6H4; R2 = H, Ph; R3 = H, HO) were prepd. Thus,
AΒ
     7-hydroxy-2,3-diphenylchromone was treated with epichlorohydrin to give
     7-(2,3-epoxypropoxy)-2,3-diphenylchromone, which was treated with Me2CHNH2
     to give the chromone II. II had antihypertensive activity at 8 mg/kg in
     the spontaneously hypertensive rat.
     chromone aminohydroxypropoxy; antihypertensive aminohydroxypropoxychromone
ST
     Antihypertensives
ΙT
         ((aminohydroxypropoxy)chromone)
                                                                 84858-25-3P
                                                  84858-23-1P
                                   84858-22-0P
                    76323-05-2P
                                                                  84858-32-2P
      38186-01-5P
                                                  84858-31-1P
IT
                                   84858-30-0P
                    84858-28-6P
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      84858-27-5P
                                                   84858-39-9P
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      84858-34-4P
                                    84858-45-7P
                     84858-44-6P
      84858-43-5P
      RL: BAC (Biological activity or effector, except adverse); BSU (Biological
                                    84858-57-1P
      study, unclassified); SPN (Synthetic preparation); BIOL (Biological
      study); PREP (Preparation)
          (prepn. and antihypertensive activity of)
      RL: SPN (Synthetic preparation); PREP (Preparation)
      37933-96-3P
 ΙT
          (prepn. and reaction of isopropylamine)
                                                                  84858-60-6P
                                                   84858-48-0P
                                    84858-46-8P
                     84858-21-9P
      84858-19-5P
 IT
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
       (Reactant or reagent)
          (prepn. and reaction with isopropylamine)
       RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 IT
```

(Reactant or reagent)
(prepn. and reaction with isopropylamines)
TT 84858-42-4P

84858-42-4P RL: SPN (Synthetic preparation); PREP (Preparation)

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(prepn. and reactions with isopropylamine)
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                  84858-20-8P
                                 84858-24-2P
IT
     84858-18-4P
                                               84858-53-7P 84858-54-8P
     84858-35-5P
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     84858-56-0P 84858-58-2P
                                 84858-59-3P
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        (prepn. of)
                           1003-03-8
TΤ
                627-35-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with (epoxypropoxy)diphenylchromone)
     75-04-7, reactions 107-10-8, reactions 109-73-9, reactions
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IT
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        (reaction of, with (epoxypropoxy) flavone)
     75-31-0, reactions
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with (epoxypropyl)chromones)
                             6665-86-7 13057-72-2
                                                    18651-11-1
ΙT
     2859-88-3
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     18651-15-5
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     84858-65-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with epichlorohydrin)
ΙT
     106-89-8, reactions
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        (reaction of, with hydroxychromones)
     84858-26-4
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with isopropylamine)
TT
     13057-72-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with epichlorohydrin)
     13057-72-2 HCAPLUS
RN
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
CN
                Ph
    ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2003 ACS
L50
     1981:550452 HCAPLUS
ΑN
DN
     95:150452
     Basic ethers and pharmaceutical preparations containing them
ΤI
     Hausberg, Hans Heinrich; Pruecher, Helmut; Uhl, Juergen; Seyfried,
ΙN
     Christoph; Minck, Klaus
     Merck Patent G.m.b.H. , Fed. Rep. Ger.
PΑ
     Ger. Offen., 41 pp.
SO
     CODEN: GWXXBX
DT
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     German
T.A
     C07D311-36; C07D311-20; C07D311-22; C07D311-30
TC
     27-17 (Heterocyclic Compounds (One Hetero Atom))
CC
     Section cross-reference(s): 26
FAN.CNT 1
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                                            DE 1979-2950135
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                       Α1
     EP 31885
     EP 31885
                     В1
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R: AT, BE, CH, DE, FR, GB, IT, NL, SE

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AT 1980-107005
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    AT 8141
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                                             CA 1980-366689
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    CA 1154444
                                                                19801212 <--
                                             IL 1980-61698
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                             19850929
     IL 61698
                                                                19801213 <---
                                             HU 1980-2975
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                             19830530
     HU 25083
                        В
                             19840428
     HU 183265
                                                                19801215 <--
                                             US 1980-216454
                             19830308
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     US 4376123
                                                                19830121 <--
                                              US 1983-459928
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                        Α
     US 4508732
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                                                                19861106 <--
                              19881025
     US 4780478
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                              19791213
PRAI DE 1979-2950135
                              19801113
                                        <--
     EP 1980-107005
                                        <--
                              19801215
     US 1980-216454
                              19830121
                                        <--
     US 1983-459928
                              19850211
     US 1985-700226
GΙ
```

Basic ethers I (R = MeNR2CH2CH2CHR1, Q, Q1, Q2; R1 = cyclopropyl, R5; R2 = H, C1-4 alkyl, C2-4 alkenyl, C4-8 cycloalkylalkyl, PhCH2; R3 = H, R5; R4 = AB H, C1-4 alkyl; R5 = Ph, optionally substituted with F, C1, C1-4 alkoxy or alkylthio, OCH2O, CF3; X = OCHR6CHR7CH2, OCHR6CHR7CO, OCR6:CR7CO, CH2CHR6CHR7CO; R6, R7 = H, C1-4 alkyl, C3-6 cycloalkyl, R5), useful as antidepressants (no data), were prepd. A soln. of 7-hydroxyisoflavone in ethanolic KOH was evapd. and the residue in DMF treated with PhCHClCH2CH2NMe2 in DMF at 150.degree. to give (aminopropoxy)isoflavone

amino ether antidepressant prepn; isoflavone aminopropoxy antidepressant ST prepn; aminopropoxyisoflavone antidepressant prepn

Antidepressants ΙT

(amino ethers)

13057-72-2 IT

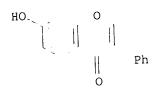
RL: PROC (Process)

(conversion of, to potassium salt)

79130-67-9P IT

```
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and debenzylation of)
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
ΙT
        (prepn. and reaction of, with aminochloropropane deriv.)
     (Reactant or reagent)
                                                              79130-57-7P
                                 79130-55-5P
                                                              79130-62-4P
                   79130-54-4P
     79130-52-2P
                                                79130-61-3P
                                  79130-60-2P
TT
                   79130-59-9P
                                                              79130-68-0P
                                                79130-66-8P
     79130-58-8P
                                  79130-65-7P
                                                              79130-73-7P
                   79130-64-6P
                                                79130-72-6P
     79130-63-5P
                                  79130-71-5P
                                                              79130-78-2P
                   79130-70-4P
                                                79130-77-1P
     79130-69-1P
                                  79130-76-0P
                   79130-75-9P
                                                              79130-83-9P
                                                79130-82-8P
     79130-74-8P
                                  79130-81-7P
                                                               79130-88-4P
                   79130-80-6P
                                                79130-87-3P
     79130-79-3P
                                  79130-86-2P
                                                               79130-94-2P
                    79130-85-1P
                                                79130-93-1P
     79130-84-0P
                                  79130-91-9P
                                                               79130-99-7P
                    79130-90-8P
                                                79130-98-6P
     79130-89-5P
                                  79130-97-5P
                    79130-96-4P
     79130-95-3P
                    79137-17-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
                                                          79131-04-7
         (prepn. of)
                                              79131-03-6
                                79131-02-5
                                           79131-08-1 79131-09-2
                   79131-01-4
      79131-00-3
                              79131-07-0
 IT
      79131-05-8 79131-06-9
                                                           79131-14-9
                                              79131-13-8
                                 79131-12-7
                   79131-11-6
      79131-10-5
                                 79137-18-1
                   79131-16-1
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (reaction of, with aminohalo compd.)
                    79131-18-3
      RL: RCT (Reactant); RACT (Reactant or reagent)
 ΙT
          (reaction of, with aminopropyl chloride deriv.)
       RL: RCT (Reactant); RACT (Reactant or reagent)
  TT
          (reaction of, with hydroflavone sodium salt)
       RL: RCT (Reactant); RACT (Reactant or reagent)
  IT
          (reaction of, with hydroxychroman sodium salt)
                             5911-08-0
       106-95-6, reactions
       RL: RCT (Reactant); RACT (Reactant or reagent)
  ΙT
          (N-alkylation by, of (aminopropoxy)isoflavone deriv.)
       RL: RCT (Reactant); RACT (Reactant or reagent)
  IT
           (N-methylation of)
        RL: RCT (Reactant); RACT (Reactant or reagent)
   TΤ
           (O-alkylation by, of hydroxyisoflavone)
        13057-72-2
   IT
        RL: PROC (Process)
           (conversion of, to potassium salt)
        4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
        13057-72-2 HCAPLUS
   RN
   CN
   HO_
              0
                    Ph
               0
         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    IT
             (prepn. and reaction of, with aminochloropropane deriv.)
         (Reactant or reagent)
          79130-53-3 HCAPLUS
    RN
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4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl-, potassium salt (9CI) (CA CN INDEX NAME)



K

79131-06-9 ΙT

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with aminohalo compd.)

4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl-, sodium salt (9CI) (CA INDEX 79131-06-9 HCAPLUS RNCN NAME)



Na

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L50 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2003 ACS
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1980:6415 HCAPLUS AN

92:6415 DN

Animal feed containing anabolic isoflavones

Feuer, Laszlo; Nogradi, Mihaly; Gettsegen, Agnes; Vermes, Borbala; Strelisky, Janos; Wolfner, Andras; Farkas, Lorant; Antus, Sandor; Toth, TIIN Maria K.

Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt., USA

U.S., 8 pp. Cont.-in-part of U.S. 3,833,730. PASO

CODEN: USXXAM

DTPatent

English LA

A61K031-35 IC

NCL 424283000 27-15 (Heterocyclic Compounds (One Hetero Atom)) Section cross-reference(s): 18

Section cross-reference(s): 10										
FAN.CNT 3 PATENT NO.		KIND	DATE		APPLICATION NO.	DATE				
PI PRA	US 4166862 US 3833730 US 3907830 US 3864362 US 3949085 US 1971-146773 HU 1970-CI996	A A A A	19790904 19740903 19750923 19750204 19760406 19710525 19700527	< <	US 1974-470444 US 1971-146773 US 1973-371560 US 1973-374056 US 1974-497644	19740516 < 19710525 < 19730619 < 19730627 < 19740815 <				

```
US 1973-371560
                                19730619 <--
         7-Hydroxy-2-methylisoflavone and 7-hydroxyisoflavone ethers, which were
    AB
         prepd. from 2,4-dihydroxyphenyl benzyl ketone 4-ethers, showed their
         effectiveness as animal feed wt.-gaining additives. A mixt. of
        2,4-HO(Me2CHO)C6H3COCH2Ph, HC(OEt)3, morpholine, and DMF was refluxed 8 h,
        with removal of the EtOH formed, to give 7-isopropoxyisoflavone.
        alkoxyisoflavone prepn animal growth; benzoyloxyisoflavone prepn animal
        growth; isoflavone alkoxy prepn animal growth
   TΤ
            (additives for, hydroxyisoflavone ethers as)
        Animal growth substances
        RL: RCT (Reactant); RACT (Reactant or reagent)
           (hydroxyisoflavone ethers)
   TΤ
        557-21-1
        RL: RCT (Reactant); RACT (Reactant or reagent)
           (cyclocondensation reaction of hydrogen cyanide from, with
           o-hydroxyphenyl benzyl ketones)
   ΙT
        72111-19-4
       RL: RCT (Reactant); RACT (Reactant or reagent)
           (cyclocondensation reaction of, with acetic anhydride, isoflavone
          deriv. from)
  ΙT
       18439-96-8
       RL: RCT (Reactant); RACT (Reactant or reagent)
          (cyclocondensation reaction of, with ethoxalyl chloride)
  IT
       50561-04-1
       RL: RCT (Reactant); RACT (Reactant or reagent)
                                  50775-76-3
          (cyclocondensation reaction of, with orthoformate ester)
  TΤ
       68-12-2, reactions
       RL: RCT (Reactant); RACT (Reactant or reagent)
          (cyclocondensation reaction of, with o-hydroxyphenyl benzyl ketone
          deriv.)
       109-94-4
                  122-51-0
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (cyclocondensation reaction of, with o-hydroxyphenyl benzyl ketones)
 IΤ
      4755-77-5
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          (cyclocondensation reaction of, with o-hydroxyphenyl benzyl ketones,
         decarboxylation in)
 ΙT
      108-24-7
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (cyclocondensation reaction of, with o-hydroxyphenyl benzyl ketones,
         isoflavones from)
 ΙT
      54585-89-6P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
         (prepn. and dehydration of)
TΥ
      35212-47-6P
                    35212-50-1P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
         (prepn. and sapon. of)
ΙT
     35212-22-7P
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                                                35212-33-0P
     35212-42-1P
                                                              35212-35-2P
                   35212-52-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and use of, in animal feed)
ΙT
     844-95-1P 23915-78-8P
                               35212-24-9P
                                              35212-25-0P
     35212-29-4P
                                                            35212-26-1P
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     35212-43-2P
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                   35212-44-3P
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     RL: SPN (Synthetic preparation); PREP (Preparation)
                                               35212-46-5P
                                                              35294-02-1P
        (prepn. of)
TΤ
     13057-73-3
                  54528-15-3
                               54528-35-7
    RL: RCT (Reactant); RACT (Reactant or reagent)
                                            54528-37-9
                                                          54528-40-4
        (use of, in animal feed)
```

```
2859-88-3 13057-72-2
TΤ
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of)
     111-25-1 3145-86-6
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of hydroxyisoflavone by)
     100-44-7, reactions
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of hydroxyisoflavone deriv. by)
     78-76-2
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of hydroxyisoflavones by)
     13057-72-2
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of)
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
RN
CN
HO.
           0
                Ph
           0
 L50 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2003 ACS
     1977:405809 HCAPLUS
 AN
      4-Oxo-4H-benzopyran derivatives useful in fodder compositions
 DN
 TI
      Bass, Robert John
 ΙN
      Pfizer Corp., Panama
 PΑ
      Ger. Offen., 20 pp.
 SO
      CODEN: GWXXBX
 DT
      Patent
      German
 LA
      C07D311-36
 IC
      27-14 (Heterocyclic Compounds (One Hetero Atom))
 CC
      Section cross-reference(s): 18
 FAN.CNT 1
                                          APPLICATION NO. DATE
                       KIND DATE
      PATENT NO.
                                           _____
                             _____
      _____
                                          DE 1976-2640617 19760909 <--
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                       A1
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                                          BE 1976-170560
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A 19770315
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                                           NL 1976-10059
      NL 7610059
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                                            JP 1976-108684
                       A2 19770511
A1 19770527
       JP 52057182
                                                            19760910 <--
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       FR 2329269
                                            US 1977-795652 19770510 <--
                            19780926
                       A
       US 4117149
                             19750912 <--
  PRAI GB 1975-37553
                             19760813 <--
       US 1976-714086
```

GI

```
Benzopyranones (I; R = H, OH, Me, MeO; R1 = H, C1, OH; R2 = H, OH, Me,
     MeO; R3 = e.g. Ph, 4-MeC6H4, 4-PhC6H4, PhSO2, PhCH2, 4-MeOC6H4O,
AΒ
     cyclopentyl, 2-naphthyl), useful as animal growth substances, are prepd.
     by reaction of 2'-hydroxyacetophenones with DMF or MeCONMe2 in presence of
     MeSO2Cl and BF3.Et2O. Thus, reaction of 2,4,6-(HO)3C6H2COCH2C6H4Me-4 with DMF 2 h at 100.degree. gives 85% I (R = R2 = OH, R1 = H, R3 = 4-MeC6H4).
     benzopyranone animal growth prepn
ST
     Animal growth substances
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (benzopyranone derivs.)
     485-72-3P 491-80-5P 4044-00-2P 13057-72-2P
                                                                 59108-72-4P
IT
                                                  59108-71-3P
                                  15584-09-5P
                    15584-08-4P
     15584-07-3P
                                                                 62845-08-3P
                                                  62845-07-2P
                                   59297-07-3P
                    59108-74-6P
     59108-73-5P
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                    62845-10-7P
     62845-09-4P
                                                                 62845-18-5P
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      62845-19-6P 62845-20-9P 62845-21-0P
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                   62881-64-5P
      62845-23-2P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of)
      124-63-0
ΙT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of hydroxyacetophenone derivs. with dimethylformamide or
         dimethylacetamide in presence of borontrifluoride etherate and)
      109-63-7
ΙT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of hydroxyacetophenone derivs. with dimethylformamide or
         dimethylacetamide in presence of methanesulfonyl chloride and)
      127-19-5
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction with (fluorophenyl)trihydroxyacetophenone)
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (reaction with dimethylacetamide)
      59108-68-8
 IT
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          (reaction with dimethylformamide)
      68-12-2, reactions
 IT
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          (reaction with trihydroxytolylacetophenone)
       4044-00-2P 13057-72-2P 62845-20-9P
 IT
       62845-21-0P
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       (prepn. of)
4044-00-2 HCAPLUS
       4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-phenyl- (9CI) (CA INDEX NAME)
  RN
  CN
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13057-72-2 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME) CN

62845-20-9 HCAPLUS RN

4H-1-Benzopyran-4-one, 5-hydroxy-3-(4-hydroxyphenyl)-7-methyl- (9CI) (CA CN INDEX NAME)

62845-21-0 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-5-methyl- (9CI) (CA CN INDEX NAME)

L50 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2003 ACS

1975:16704 HCAPLUS ΑN

82:16704 DN

Catabolic 7-alkoxyisoflavones as feed additives

ΤI Feuer, Laszlo; Nogradi, Mihaly; Gottsegen, Agnes; Vermes, Borbala; Streliszky, Janos; Wolfner, Andras; Farkas, Lorant; Antus, Sandor; Kovacs, ΙN

Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt. PΑ

Ger. Offen., 23 pp. Division of Ger. Offen. 2,125,245 (CA 76: 72407e). SO CODEN: GWXXBX

DTPatent

German LA

A61K; A23K IC

27-15 (Heterocyclic Compounds (One Hetero Atom)) CC Section cross-reference(s): 5

FAN.CNT 3 PATENT	NO. KIND	DATE	API	PLICATION NO.	DATE	
PI DE 2166		19741003	DE	1971-2166458	19710521	<
HU 1623		19730228		1970-CI996	19700527	
IL 3692		19751015		1971-36929	19710520	
DE 2166	-	19730222	DE	1971-2166085	19710521	<
DE 2166		19790816				
DE 2166	_	19800424				
AT 3113		19731112		1971-444	19710524	
AT 3117		19731210		1971-10281	19710524	
AT 3186		19741111		1972-6909	19710524	
ES 3914		19750301		1971-391486	19710524	
NL 7107		19711130	NL	1971-7128	19710525	<
NL 1705		19820616				
NL 1705		19821116	2.7	1071 6745	19710525	/
SE 3890		19761025		1971-6745	19710525	
SU 4021		19731012		1971-1667729	19710526	
GB 1360		19740717		1971-17293	19710526	
GB 1360		19740717		1974-1583 1974-6068	19710526	
CH 5657		19750829		1971-7704	19710526	
CH 5674		19751015		1971-1717079	19710526	
SU 5082		19760325 19760430		1971-160121	19710526	
PL 8499		19760430		1971-1986	19710526	
NO 1342		19780227		1971-2543	19710526	
DK 1373		19780531		1971-148411	19710526	
PL 9859		19780630		1971-175267	19710526	
PL 9903	-	19720324		1971-19257	19710527	
FR 2100 CS 1578		19741015		1971-3888	19710527	
CS 165		19751222		1971-6392	19710527	<
CA 998		19761005		1971-114041	19710527	<
RO 627		19770915		1971-70509	19710527	<
JP 540		19790530		1971-35940	19710527	
FI 574		19800430	FI	1971-1463	19710527	<
FI 574	• •	19800811				
ES 398	= = :	19750416		1971-398289	19711223	
US 390		19750923		1973-371560	19730619	
US 386		19750204		1973-374056	19730627	
ES 425		19760616		1974-425900	19740502	
SE 740		19740604	SE	1974-7325	19740604	<
SE 412	586 C	19800626	_	1071 107611	10740015	. ,
US 394		19760406		1974-497644	19740815 19750110	
CA 986		19760330		1975-217729	19750110	
DK 760		19760421	DF	( 1976-1789	19/0042.	
DK 143		19810921				
DK 143		19820222	тт	2 1977-115994	1977092	7 <
JP 530		19780516	JI	1311-113334	15,1052	
JP 590		19840127	₽*	[ 1979-1702	19790528	3 <
FI 790		19790528	r.	1010 1102	10,0002	-
FI 640		19830630 19831010				
FI 640		19840410	т.	2 1982-216782	1982121	O <
JP 590		19840621	0.	2002 220.42		
JP 590 PRAI HU 197		19700527	<			
	1-146773	19710525	<			
	1-2543	19710526	<			
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	71-1463	19710527	<			
	3-371560	19730619	<			
OT 17 414	(a) coo	orinted CA T	SSUE			
AD About	40 icoflavones	[T. Rn = H]	(OMe)2	-3,4, or NO2-4	H; R1 = H,	Me, or
CO2H;	R2 = e.g. C1-1	l alkyl, PhC	CH2, 4-C	1C6H4CH2, EtO2	CCH2, HOC	HZCHZ,

ST

ΙT

IT

IT

ΙT

TΤ

IT

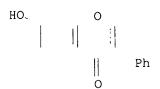
ΙT

IT

TT

TT

```
EtOCH2CH2, or 3-pyridylpropyl] were prepd. and (or) used as catabolic feed
   additives. Thus, 2,4-HO(Me2-CHO)C6H3COCH2Ph and HC(OEt)3 were refluxed in
  DMF contg. morpholine to give I (Rn = R1 = H, R2 = Me2CH).
   2,4-HO-(BuO)C6H3COCH2Ph was refluxed in Ac2O contg. AcONa to give I (Rn =
   H, R1 = Me, R2 = Bu). I (Rn = R1 = R2 = H) and hexyl bromide were
   refluxed in Me2CO contg. K2CO3 and KI to give I (Rn = R1 = H, R2 = hexyl).
   2,4-HO(MeO)C6H3CO-CH2Ph reacted with ClCOCO2Et in pyridine to give Et
   2,3-dihydro-2-hydroxy-7-methoxyisoflavone-2-carboxylate, which on heating
   with concd. HCl gave I (Rn = H, R1 = CO2Et, R2 = Me) (II). II was
   hydrolyzed in aq. NaOH and Me2CO to give I (Rn = H, R1 = CO2H, R2 = Me).
   feed additive catabolic isoflavone; alkoxyisoflavone feed additive;
   pyridylpropoxyisoflavone feed additive
   Feed
      (additives, catabolic alkoxyisoflavones as)
                                                        54528-35-7
                                           54528-15-3
                             54510-03-1
                50776-06-2
   13057-73-3
                                                        54585-86-3
                                           54528-40-4
                             54528-38-0
                54528-37-9
   54528-36-8
   RL: RCT (Reactant); RACT (Reactant or reagent)
      (catabolic feed additive)
                                                4755-77-5
                         122-51-0
                                     557-21-1
              109-94-4
   108-24-7
   RL: RCT (Reactant); RACT (Reactant or reagent)
       (cyclization of benzyl phenyl ketones and)
                            50775-76-3
                50775-75-2
   50561-04-1
   RL: RCT (Reactant); RACT (Reactant or reagent)
       (cyclization with formic acid derivs.)
                                                            35212-42-1P
                                              35212-35-2P
                                35212-33-0P
                  35212-32-9P
   35212-22-7P
   35212-52-3P
                  54851-23-9P
   RL: SPN (Synthetic preparation); PREP (Preparation)
       (prepn. and catabolic activity of)
   RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    (Reactant or reagent)
       (prepn. and dehydration of)
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    (Reactant or reagent)
       (prepn. and hydrolysis of)
                                                             35212-29-4P
                                               35212-28-3P
                                35212-26-1P
                  35212-25-0P
    35212-24-9P
                                                             35212-37-4P
                                               35212-36-3P
                                35212-34-1P
                  35212-31-8P
    35212-30-7P
                                                             35212-43-2P
                                               35212-41-0P
                                35212-40-9P
    35212-38-5P 35212-39-6P
                                               54528-34-6P
                                35294-02-1P
                  35212-51-2P
    35212-44-3P
    RL: SPN (Synthetic preparation); PREP (Preparation)
       (prepn. of)
                           54528-39-1
    2859-88-3 13057-72-2
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with alkyl halides)
    10025-87-3
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with dimethylformamide)
    18439-96-8
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with ethyl (chlorocarbonyl) formate)
                                     3145-86-6
               100-44-7
                         111-25-1
     78-76-2
IT
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with hydroxyisoflavones)
     68-12-2, reactions
TT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (with phosphoryl chloride)
     13057-72-2
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with alkyl halides)
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
RN
CN
```



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Waehaelae, Kristina; Hase, Tapio; Adlercreutz, Herman
ΑU
     Dep. Chemistry, Univ. Helsinki, Helsinki, FIN-00014, Finland
CS
     Proceedings of the Society for Experimental Biology and Medicine (1995),
SO
     208(1), 27-32
     CODEN: PSEBAA; ISSN: 0037-9727
PB
     Blackwell
DT
     Journal
LA
     English
     26-4 (Biomolecules and Their Synthetic Analogs)
CC
     The synthesis of the important diphenolic isoflavone type of
AΒ
     phytoestrogens starting from the corresponding unprotected phenols and
     arylacetic acids is discussed. The aryl rings may carry addnl. alkyl,
     methoxy, and/or halogeno groups. Intermediate polyhydroxydeoxybenzoins
     can also be isolated in good yield. Isotopically labeled isoflavone
     phytoestrogens were prepd. by H/D exchange in the complete mol. By this
     method the deuterated products are available in an isotopic purity of
     .gtoreq.90%.
     isoflavone; arylacetate phenol acylation; deuteration daidzein genistein
ST
     Flavonoids
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (iso-, oxo, prepn. and labeling of isoflavones from phenols and
        arylacetic acids)
     104-01-8, 4-Methoxyphenylacetic acid
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (prepn. and labeling of isoflavones from phenols and arylacetic acids)
                     136466-47-2P
IT
     104411-13-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and labeling of isoflavones from phenols and arylacetic acids)
                                    93-25-4, 2-Methoxyphenylacetic acid
     87-66-1, 1,2,3-Benzenetriol
IT
                                          103-82-2, Phenylacetic acid, reactions
     95-88-5, 4-Chloro-1,3-benzenediol
                                            108-46-3, 1,3-Benzenediol, reactions
     106-44-5, 4-Methylphenol, reactions
                                                                   120-80-9,
     108-73-6, 1,3,5-Benzenetriol
                                     108-95-2, Phenol, reactions
                                   156-38-7, 4-Hydroxyphenylacetic acid
     1,2-Benzenediol, reactions
     306-08-1, 4-Hydroxy-3-methoxyphenylacetic acid
                                                      504-15-4,
                                                                608 - 25 - 3,
                                 533-73-3, 1,3,4-Benzenetriol
     5-Methyl-1, 3-benzenediol
                                 614-75-5, 2-Hydroxyphenylacetic acid
     2-Methyl-1,3-benzenediol
                                             1798-09-0, 3-Methoxyphenylacetic
     621-37-4, 3-Hydroxyphenylacetic acid
     acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (prepn. of isoflavones from phenols and arylacetic acids)
                                           3669-41-8P
                                                         15485-65-1P
 16-2 487-49-08 - -217)-31-8P
                               2491-32-9P
                                                              89019-84-1P
                                                89019-83-0P
      17720-60-4P
                    40456-49-3P
                                  77316-95-1P
                                                  139256-04-5P
                                                                 150295-88-8P
                                   139256-03-4P
                    139256-02-3P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (prepn. of isoflavones from phenols and arylacetic acids)
                             485-72-3P, 7-Hydroxy-4'-methoxyisoflavone
      446-72-0P, Genistein
 IT
                            491-80-5P, 5,7-Dihydroxy-4'-methoxyisoflavone
      486-66-8P, Daidzein
                              4044-00-2P, 5,7-Dihydroxyisoflavone
                                                                     13057-72-2P,
      574-12-9P, Isoflavone
                            19725-36-1P
                                          21913-98-4P
                                                        62845-21-0P
      7-Hydroxyisoflavone
                                                                   89019-85-2P
      63909-40-0P, 7-Hydroxy-2'-methoxyisoflavone
                                                    75187-63-2P
                                   139256-06-7P 139256-07-8P
                     139256-05-6P
      118024-87-6P
      139256-08-9P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of isoflavones from phenols and arylacetic acids)
      139256-07-8P
 IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of isoflavones from phenols and arylacetic acids)
      139256-07-8 HCAPLUS
 RN
      4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI)
 CN
      INDEX NAME)
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HO.
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Cl
                       OH
           0
    ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS
L15
     1992:105915 HCAPLUS
ΑN
     116:105915
DN
ΤI
     Expedient synthesis of polyhydroxyisoflavones
     Wahala, Kristiina; Hase, Tapio A.
ΑU
     Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
CS
SO
     Journal of the Chemical Society, Perkin Transactions 1:
     Bio-Organic Chemistry (1972-1999) (1991), (12), 3005-8
     CODEN: JCPRB4; ISSN: 0300-922X
DT
     Journal
     English
LA
CC
     26-4 (Biomolecules and Their Synthetic Analogs)
os
     CASREACT 116:105915
     Polyhydroxyisoflavones (19 compds.) were prepd. by reaction of unprotected
AΒ
     phenols with arylacetic acid in the presence of BF3.Et2O followed by
     treatment with MeSO2C1. In many cases the intermediate deoxybenzoins were
     also isolated.
ST
     isoflavone polyhydroxy; deoxybenzoin polyhydroxy; phenol arylacetate
     condensation
IT
     Flavonoids
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (iso-, hydroxy oxo, polyhydroxy-, prepn. of, from unprotected phenols
        and arylacetic acids)
     1835-11-6
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidn. of)
IT
     487-49-0P
                 2491-31-8P
                               2491-32-9P
                                            3669-41-8P
                                                         15485-65-1P
                    40456-49-3P
                                  52122-86-8P
                                                77316-95-1P
                                                               89019-83-0P
     17720-60-4P
                   92549-46-7P
                                  139256-01-2P
                                                 139256-02-3P
                                                                 139256-03-4P
     89019-84-1P
     139256-04-5P
     RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (prepn. and intramol. cyclocondensation of)
IT
     306-08-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (prepn. and reaction of, with phenols)
IT
     67736-18-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of)
                                          491-80-5P
                                                      574-12-9P, Isoflavone
ΙT
     446-72-0P
                  485-72-3P
                              486-66-8P
                                                              32684-57-4P
                   13057-72-2P
                                 19725-36-1P
                                               21913-98-4P
     4044-00-2P
                                  75187-63-2P
                                                89019-85-2P
                                                               118024-87-6P
     62845-21-0P
                    63909-40-0P
                     139256-06-7P 139256-07-8P
                                                 139256-08-9P
     139256-05-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, from phenol and phenylacetic acid)
                                            103-82-2, Phenylacetic acid,
IT
     93-25-4, 2-Methoxyphenylacetic acid
                  104-01-8, 4-Methoxyphenylacetic acid
     reactions
                                   614-75-5, 2-Hydroxyphenylacetic acid
     4-Hydroxyphenylacetic acid
     621-37-4, 3-Hydroxyphenylacetic acid
                                             1798-09-0, 3-Methoxyphenylacetic
     acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
```

95-88-5, 4-Chloro-1, 3-benzenediol

(reaction of, with phenols)

87-66-1, 1,2,3-Benzenetriol

IT